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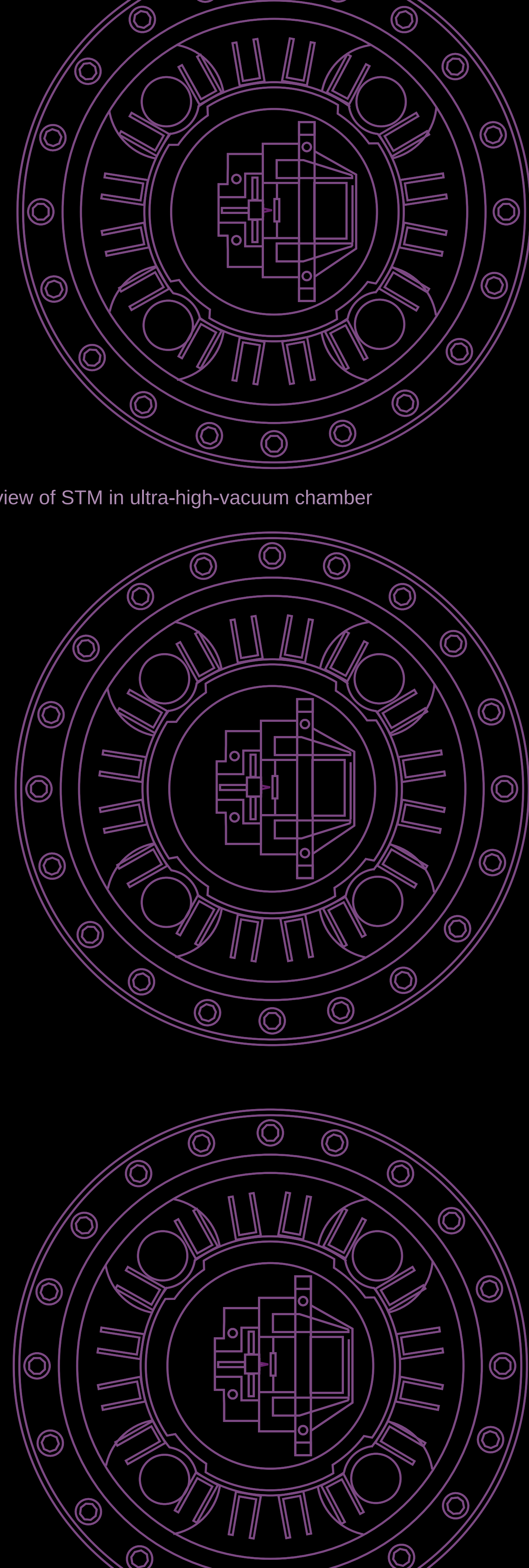

Top view of STM in ultra-high-vacuum chamber

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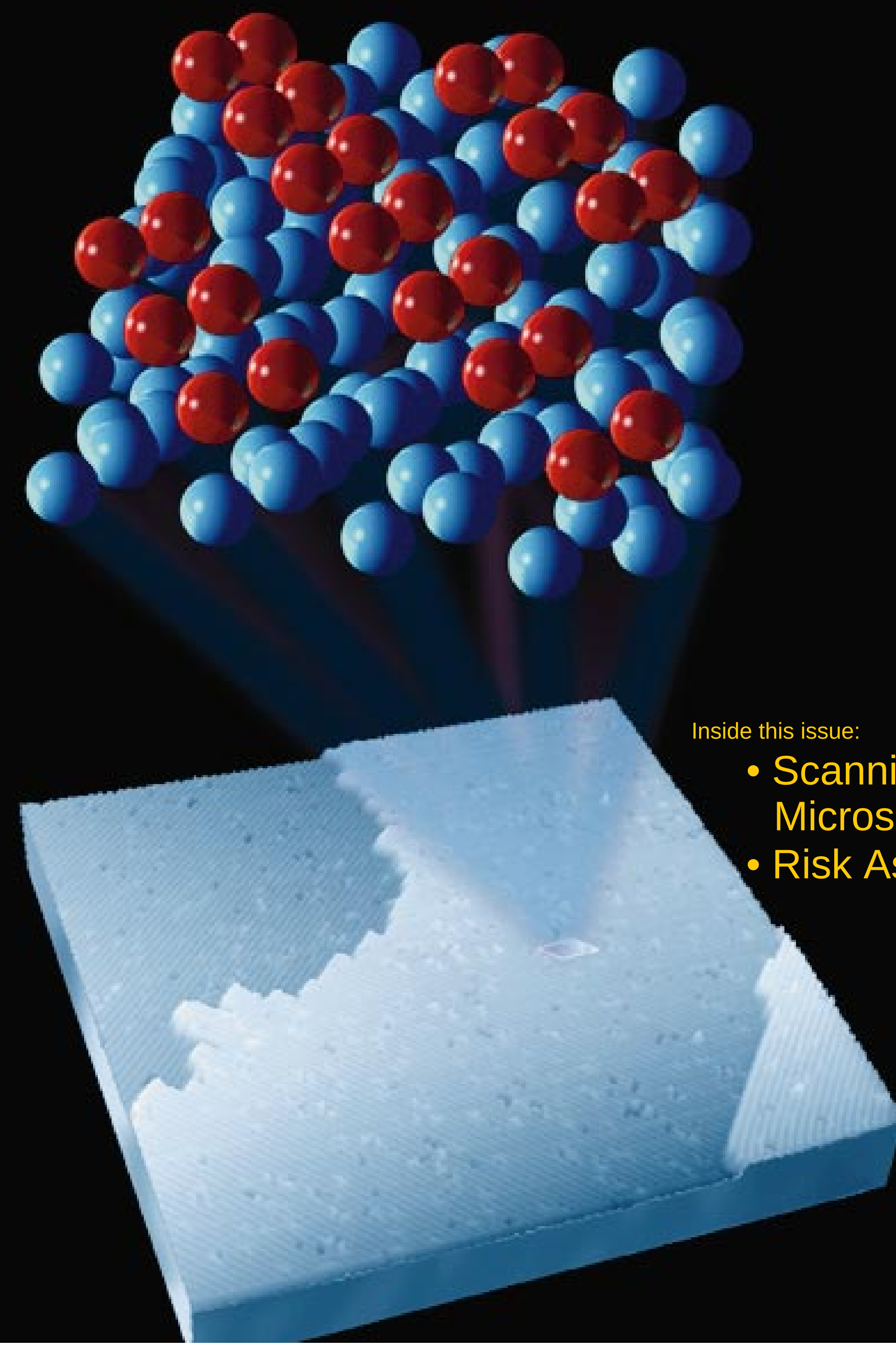

Inside this issue:

- Scanning Tunneling Microscopy
- Risk Assessment

About the Cover

The scanning tunneling microscope (STM) provides an image of the atomic arrangement of a material's surface. The rendered enlargement shows bonds formed between adjacent atoms For further information, see the feature article beginning on page 4.

Cover illustration: John Maduell

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About *S&TR*

The Lawrence Livermore National Laboratory, operated by the University of California for the United States Department of Energy, was established in 1952 to do research on nuclear weapons and magnetic fusion energy. *Science and Technology Review* (formerly *Energy and Technology Review*) is published monthly to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments, particularly in the Laboratory's core mission areas—global security, energy and the environment, and bioscience and biotechnology. Rather than just informing people of these accomplishments, the publication's goal is to help readers understand them and appreciate their value to the individual citizen, the nation, and the world.

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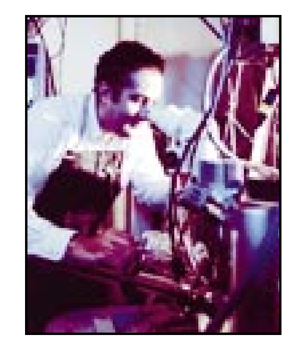

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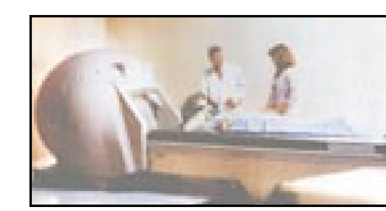

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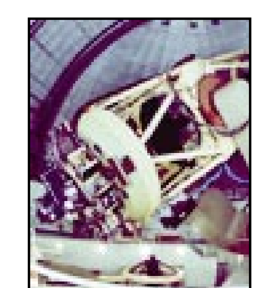

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Many applications for advanced cooling system

Laboratory scientists and industrial partners have designed a new low-power, portable, fieldable, helium-based cooling system. Originally designed for a radiation detection system, it promises to find applications in many areas, from food refrigeration to scientific instrumentation. A patent application has been filed, and the Laboratory is seeking to license the design to industrial partners.

Key to the system is the use of microprocessors to minimize vibration; they allow the compressor's motor to become more efficient, use less energy, and last longer. Instead of environmentally harmful chlorofluorocarbons, the new system uses small amounts of helium as a coolant. The design also eliminates the use of liquefied nitrogen (LN_2).

LN_2 has been a potentially hazardous component of most cooling systems that are built to deliver very low temperatures—for example, those used in radiation detection systems such as medical PET scans. Cooling systems that use liquefied nitrogen also are bulky and expensive to maintain and require extensive safety mechanisms. Thus, they have been considered impractical.

The small size, low power requirement, LN_2-free operation, and low vibration features of the Livermore cooling system are qualities researchers sought in a cooling system for a portable, fieldable radiation detector. Lab researchers expect their design to result in a number of portable, fieldable systems, including those for environmental monitoring and locating underground oil deposits.

Contact: Ken Neufeld (510) 423-8718 (neufeld@isd.llnl.gov).

Dismantlement approach seeks to reduce waste

This September, the Laboratory plans to begin a year-long technology development effort aimed at finding ways for the nation to dismantle its nuclear weapons with greatly reduced plutonium-contaminated waste. The small-scale effort to be conducted in the Laboratory's plutonium facility will use mechanical and thermal approaches for reducing waste. First, researchers plan to use a cutter that does not produce waste chips to open a plutonium pit that has been removed from a nuclear weapon. Then they will use a process called HYDEC (hydride-dehydride-cast), which uses hydrogen gas and heat to remove the plutonium and then casts it into small ingots for storage.

Plans call for processing about 20 to 25 pits from the DOE's Rocky Flats Plant during the prototype test period. Afterward, the resulting plutonium ingots will be returned there. The project could establish a more cost-effective, less time-intensive dismantlement procedure.

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Lab leads manufacturing of B Factory rf cavities

The Laboratory is directing the manufacture of all radio-frequency (rf) cavities needed for operating the B Factory accelerator and detector—sometimes known as PEP-II and BaBar. The $177-million accelerator and the $75-million detector are designed to advance understanding in the field of particle physics. Located at the Stanford Linear Accelerator Center (SLAC), the B Factory is a collaboration between SLAC and the Lawrence Berkeley and Lawrence Livermore National Laboratories.

Each cavity will be 2 ft in diameter and weigh about 450 lb. The rf cavities will be powered in pairs by a 1-megawatt microwave generator. The first cavity was shipped to SLAC on May 30 as part of a $4-million project spread over the next two years. In all, 26 additional rf cavities will be constructed. While conventional machining on the rf cavities is being contracted to U.S. industry, critical fabrication and assembly activities are centered in Livermore, where about 60 technicians and machinists are involved.

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Workshop addresses planetary defense

An international Planetary Defense Workshop was held in Livermore May 22–26, 1995. Titled "An International Technical Meeting on Active Defense of the Terrestrial Biosphere from Impact of Large Asteroids and Comets," the event attracted about 150 scientists. After reviewing present understanding of the basic nature of the threat posed by asteroid and comet impacts, attendees gathered in working groups to examine specialized issues, including detection, tracking, and categorization of threat objects, and technologies and systems for threat object deflection and dispersion.

The workshop was co-hosted by LLNL and DOE. Sponsoring organizations were LLNL, DOE, National Aeronautics and Space Administration, Los Alamos National Laboratory, Air Force Space Command, Air Force Phillips Laboratory, Naval Research Laboratory, Russian Federal Nuclear Centers VNIITF Chelyabinsk-70 and VNIIEF Arzamas-16, Makeev State Rocket Center, the Russian ministries of Energy and Defense, China's Center of Advanced Science and Technology-World Lab (Beijing), and the World Laboratory (Erice and Geneva).

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Jeffrey Wadsworth
Associate Director for Chemistry and Materials Science

THE external forces that are reshaping the Laboratory and refocusing its programs are having a significant impact on the disciplines as well. Chemistry and Materials Science, together with Physics, Engineering, and Computation, provide the disciplinary foundation for all of the Laboratory's programs. In many respects, recent changes are beneficial, particularly because they help us to sharpen our mission and purpose as a discipline.

Chemistry and Materials Science plays a vital role in the success of Laboratory programs. Lasers, weapons, nonproliferation, environmental remediation, energy technologies, advanced manufacturing, structural biology—these programs and others all involve challenging aspects of chemistry and materials science. We must provide the core-discipline expertise to meet the objectives of existing programs, plus we must continue to advance the state of the art in order to create the scientific foundations for new and evolving programs.

Our role is to be a supporting partner to existing and evolving Laboratory programs. By assigning personnel through our matrix system, we provide the programs with the required mix of scientific skills in chemistry and materials science, as well as with individuals to assist in technical project management. To this end, it is essential that we forecast accurately the types of scientific talent needed and that we attract and retain the best scientists in those areas. Given current uncertainties regarding Laboratory missions and program directions, scientific flexibility and breadth of interest are increasingly important.

Synergy between the programs and disciplines is responsible for much of the Laboratory's success over the years. Fundamental scientific discoveries open the doors to new programs, and programmatic requirements push the state of the art in the disciplines. The article in this issue on scanning tunneling microscopy is an excellent example of this process. Many programs require ever-more detailed imaging methods—electronics engineers need to be able to fabricate microcircuit patterns a few tens of atoms thick, biologists want to study single molecules of protein or DNA, and materials scientists need to be able to examine atomic-scale flaws in crystals or coatings. As scanning tunneling microscopy and atomic-force microscopy have evolved, these tasks become possible.

Indeed, one of our most difficult challenges is deciding which exciting innovations to pursue because the creativity of our scientists far exceeds our resources. Only through close partnership with the programs can we understand and anticipate their chemistry and materials science needs. And as we structure our research to develop the new processes, materials, and characterization techniques that will be needed, we make the scientific and technical discoveries that lead to new programs. Examples include the development of nanoengineered materials (aerogels and multilayers) and new processes for forming ceramic–metal composites. In these ways, the disciplines participate in and influence the evolution of the Laboratory's programs.

Guiding the development of new disciplinary capabilities and innovations is especially challenging at a time when national expectations of our Laboratory are changing rapidly. Regardless of how the Laboratory and its programs evolve, chemistry and materials science will play a key role. We are doing all that is possible to provide the right people and the research environment to foster the continual advancement of our technical capabilities and to sow the intellectual seeds for new program directions.

Scanning Tunneling Microscopy:

Opening a New Era of Materials Engineering

Spectacular advances in the development of artificial materials—now engineered on the nanometer scale—have spurred the parallel development of new tools to characterize surface and interfacial structure at the atomic scale. Our surface physics facility applies ultra-high-vacuum scanning tunneling microscopy to accelerate the development of such advanced materials.

IN the last decade, the ability of materials scientists to "nanoengineer" artificial materials—to build materials atom by atom with a predetermined arrangement and goal—has enabled the development of new technologies with applications that range from the spectacular to the mundane.[1,2] For example, x-ray mirrors composed of alternating, thin (less than 20-nanometer) films of molybdenum and silicon constitute the optics that are used to produce high-resolution pictures of the sun. Optoelectronic components composed of alternating atomic layers of different elements are the devices that enable us to extract information from video compact disks and to generate and detect transoceanic telephone signals by fiberoptic cables. The alternating, ultrathin layers of cobalt and iron in new high-density magnetic storage heads, and increasingly miniature microelectronics, are fundamental constituents of powerful desktop computers, portable laptops, and pocket-size wireless telephones.

The smaller these devices become, the more their performance depends on the atomic ordering of their constituent materials. Such details include the arrangement of atoms in crystal structures and the presence, size, and density of grain boundaries, impurities, dislocations, or other imperfections. Enhanced performance of a device—increased reflectivity in the case of x-ray mirrors, efficiency in the case of optoelectronics, switching speed in the case of transistors for microelectronics, and hardness in the case of high-strength coatings—therefore depends critically on the precise control of the details of atomic ordering during manufacture. This is where LLNL's surface physics facility in the Chemistry and Material Science Directorate enters the picture with its ultra-high-vacuum scanning tunneling microscopy capabilities.

Analyzing Atomic Arrangement

To diagnose the effect of atomic arrangement on material performance, materials scientists use a battery of techniques. Traditionally, diffraction-based probes have been the mainstay of structural analysis, and have provided most of our basic knowledge about the atomic arrangement of materials. In diffraction, a beam of light or particles (neutrons, electrons, etc.) is scattered from an object, and the three-dimensional, geometric distribution of the scattered rays is determined by the structure of the object. For example, the pattern of visible light reflected from the surface of an audio compact disc held under bright light indicates the spacing of bits written onto the disc. Similarly, the diffraction of beams of a wavelength that is comparable to the spacing between atoms in a crystal indicates the spacing between the atoms.

X-ray diffraction, the primary tool for analyzing the long-range, atomic ordering of solids, enabled the development of crystallography and provided the experimental data from which the structure of DNA was deduced. Transmission electron microscopy, another diffraction-based tool, is often used to provide images of imperfections in crystals. In both x-ray diffraction and transmission electron microscopy, however, diffraction measurements reveal the internal atomic arrangements of a material only when crystalline order extends over at least several hundred atomic spacings; in this case the material is said to exhibit "long-range" order. In contrast, when crystalline order exists over shorter distances, the material is said to exhibit "short-range" order, which may not be detected by diffraction.

Analyzing Surface Structure

These two diffraction techniques present the "bulk," or three-dimensional, atomic arrangement of a material. In nanoengineering, however, we must control how the individual atomic layers of material are deposited. Because the structural integrity of each atomic layer depends critically on the detailed atomic ordering of the surface upon which it is deposited, we must be able to "see" the atomic ordering, or structure, of that surface. To do this, we need a separate class of diagnostics that presents the two-dimensional atomic arrangement of the outermost layer of atoms in a material, rather than its three-dimensional bulk structure.

Low-Energy Electron Diffraction

For many years, the characterization of surface structure has relied on the diffraction of electrons of low energy (fewer than 200 V). Because such low-energy electrons do not penetrate beyond a few atomic layers into a crystal, their diffraction from a crystal yields the long-range atomic order on a surface. Although low-energy electron diffraction is responsible for most of our current knowledge of surface crystallography, it cannot reveal the short-range crystalline order of nanometer-scale dimensions. Yet it is on this very scale that clusters of deposited atoms initially aggregate, or nucleate, and influence the atomic arrangement of subsequently grown material. In this regime, true atomic resolution is necessary, and the scanning tunneling microscope is indispensable.

Scanning Tunneling Microscopy

The scanning tunneling microscope[3] (STM) provides a picture of the atomic arrangement of a surface by sensing corrugations in the electron density of the surface that arise from the positions of surface atoms (see Figure 1). A finely sharpened tungsten wire (or "tip") is first positioned within 2 nanometers of the specimen by a piezoelectric transducer, a ceramic positioning device that expands or contracts in response to a change in applied voltage. This arrangement enables us to control the motion of the tip with subnanometer precision. At this small separation, as explained by the principles of quantum mechanics, electrons “tunnel” through the gap, the region of vacuum between the tip and the sample. If a small voltage (bias) is applied between the tip and the sample, then a net current of electrons (the “tunneling current”) flows through the vacuum gap in the direction of the bias. For a suitably sharpened tip—one that terminates ideally in a single atom—the tunneling current is confined laterally to a radius of a few tenths of a nanometer. The remarkable spatial resolution of the STM derives from this lateral confinement of the current.

Next, additional piezoelectric transducers are used to raster the tip across a small region of the sample. As the tip scans the surface, corrugations in the electron density at the surface of the sample cause corresponding variations in the tunneling current. By detecting the very fine changes in tunneling current as the tip is swept across the surface, we can derive a two-dimensional map of the corrugations in electron density at the surface.[4] Procedures for synthesizing various nanoengineered materials often involve depositing the atoms onto a surface in such a way that the surfaces remain free of contamination. The use of ultra-high vacuum enables the preparation and atomic-resolution imaging of atomically clean surfaces, which would otherwise be contaminated immediately in air.

That is why we integrated a scanning tunneling microscope into an ultra-high-vacuum environment that includes facilities for the preparation and maintenance of atomically clean surfaces, as well as sources of the material to be deposited. We also integrated complementary, conventional surface diagnostics equipment, such as a low-energy electron diffraction probe, into this environment. The latter measures the long-range order on a surface, and STM presents the short-range order that otherwise might not be detected. In this environment, the STM offers a new opportunity for direct diagnosis of how the processing conditions affect the atomic details of surfaces.

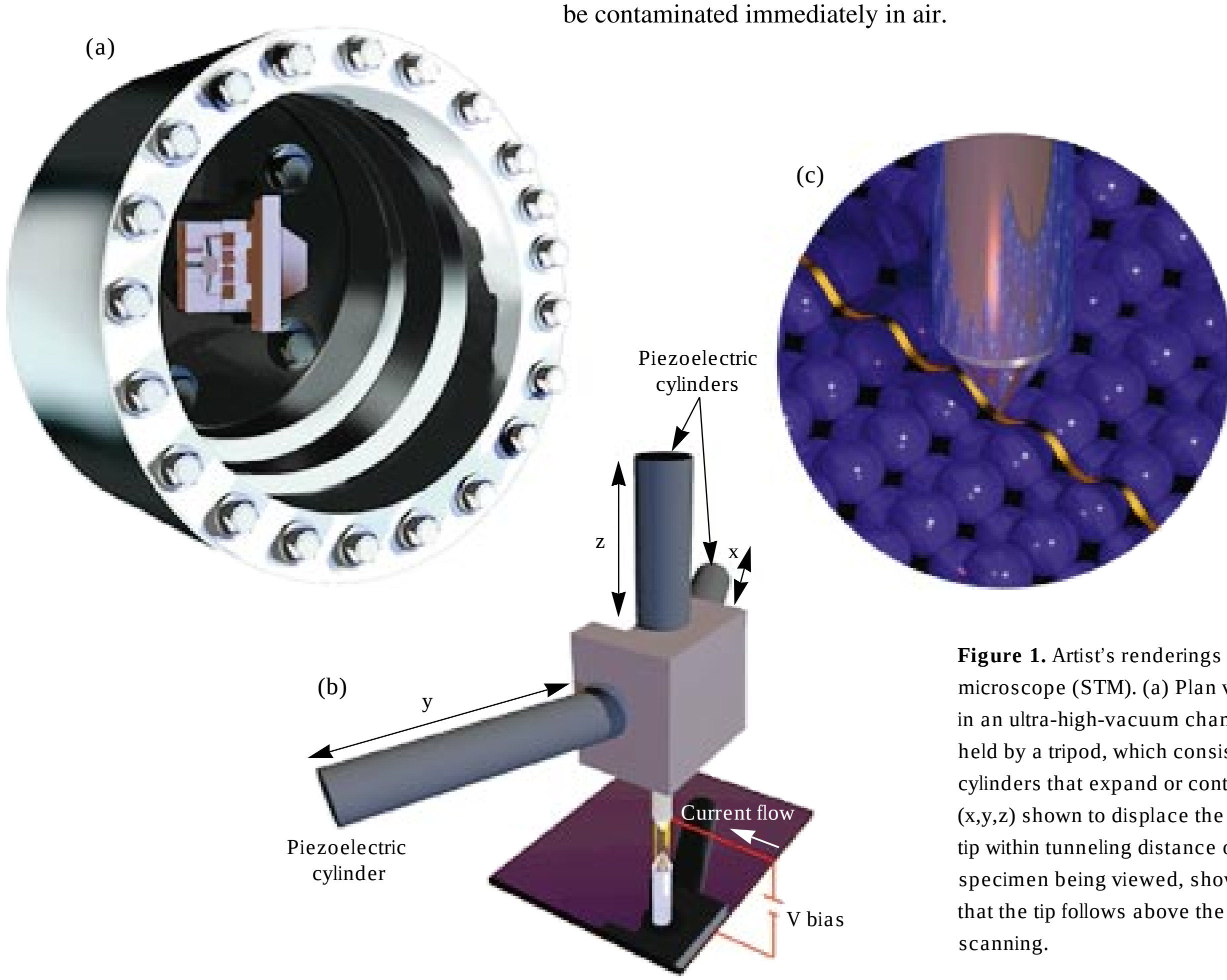


Figure 1. Artist's renderings of a scanning tunneling microscope (STM). (a) Plan view of the STM mounted in an ultra-high-vacuum chamber. (b) The probe tip as held by a tripod, which consists of three piezoelectric cylinders that expand or contract in the directions (x,y,z) shown to displace the tip. (c) A close-up of the tip within tunneling distance of the surface of the specimen being viewed, showing the ribbon-like path that the tip follows above the surface atoms during scanning.

How the Molybdenum–Silicon Interface Forms

Recently, we used this combination of surface diagnostics to study the structural development of thin films (films from one atom to several tens of nanometers thick) resulting from depositing molybdenum atoms on atomically clean silicon substrates. The data from this study can be used to develop new processes for synthesizing films that can achieve higher performance for particular applications.

For example, multilayer x-ray mirrors composed of alternating, 5- to 20-nanometer-thick layers of molybdenum and silicon achieve the best reflectivity when the interfaces between molybdenum and silicon are most abrupt—that is, when pure molybdenum is separated from pure silicon by a perfectly flat plane. However, molybdenum and silicon tend to react to form crystalline compounds, or interfacial silicides, which may adopt a variety of distinct crystal structures called phases. Because these silicides degrade this interfacial abruptness, we are trying to define processing conditions that minimize the amount of interfacial silicide.

However, molybdenum silicides also appear in other applications, such as high-temperature coatings and diffusion barriers for interconnects in very large-scale integrated circuits. For these applications, it may be desirable *not* to minimize the amount of interfacial silicide but rather to *maximize* the amount of a particular silicide phase, which may lead to enhanced performance. Our analysis is therefore intended to provide a broad correlation between the processing conditions (for example, substrate temperature and deposition rate) and the microstructural details of the resulting films, which ultimately determine how well the device will perform for a specific application. We have found that film morphology—characteristics such as roughness, crystalline structure, and grain size and orientation—depends strongly on small structures called precursors. These structures form during the initial stages of film growth and can only be detected with scanning tunneling microscopy.[5]

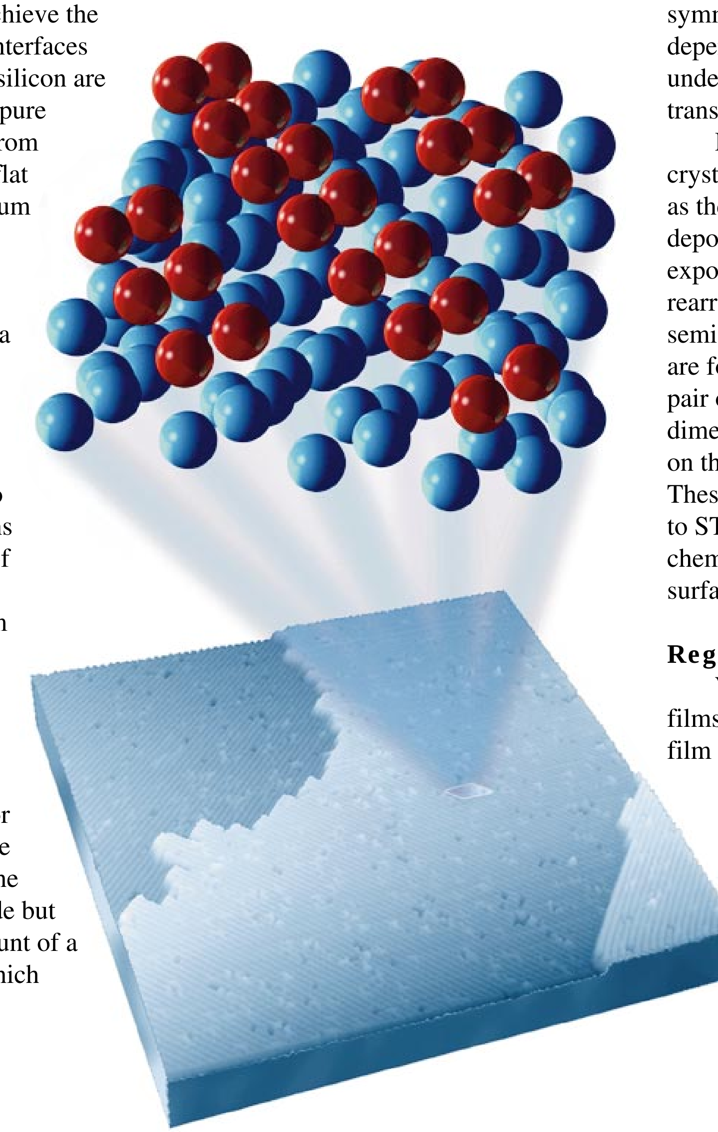


Figure 2. (Below) A 650-angstrom (Å) STM image of the surface Si(100), in which each stripe represents a row of dimers. (Above) Illustration of the atomic structure of the Si(100) surface. The outermost, dimerized atoms that contribute to the STM image below are shown in red in the illustration above.

Phases and Atomic Compositions

This reaction between molybdenum and silicon exhibits a particularly rich variety of phases and relative compositions of molybdenum and silicon, such as $MoSi_2$ and Mo_3Si. The structure of disilicide thin films, as opposed to bulk crystals, is further complicated by interfaces—both the silicide/substrate interface and the silicide surface itself. For example, there is a thin disilicide film phase that exhibits hexagonal symmetry that does not even appear in the bulk phase. Furthermore, the precise temperature at which this phase transforms to the equilibrium phase of tetragonal symmetry appears to be highly process dependent. The STM can help us understand these phases and transformations.

For example, we used the surface of crystalline silicon—designated Si(100)—as the starting substrate for film deposition. When clean Si(100) is exposed, the atoms of the surface are rearranged—as is the case with most semiconductor materials. In fact, bonds are formed between adjacent atoms, each pair of which is called a “dimer.” The dimers then align themselves into rows on the surface, as shown in Figure 2. These surface structures are important to STM studies that seek to extract chemical information about a particular surface (see box on page 8).

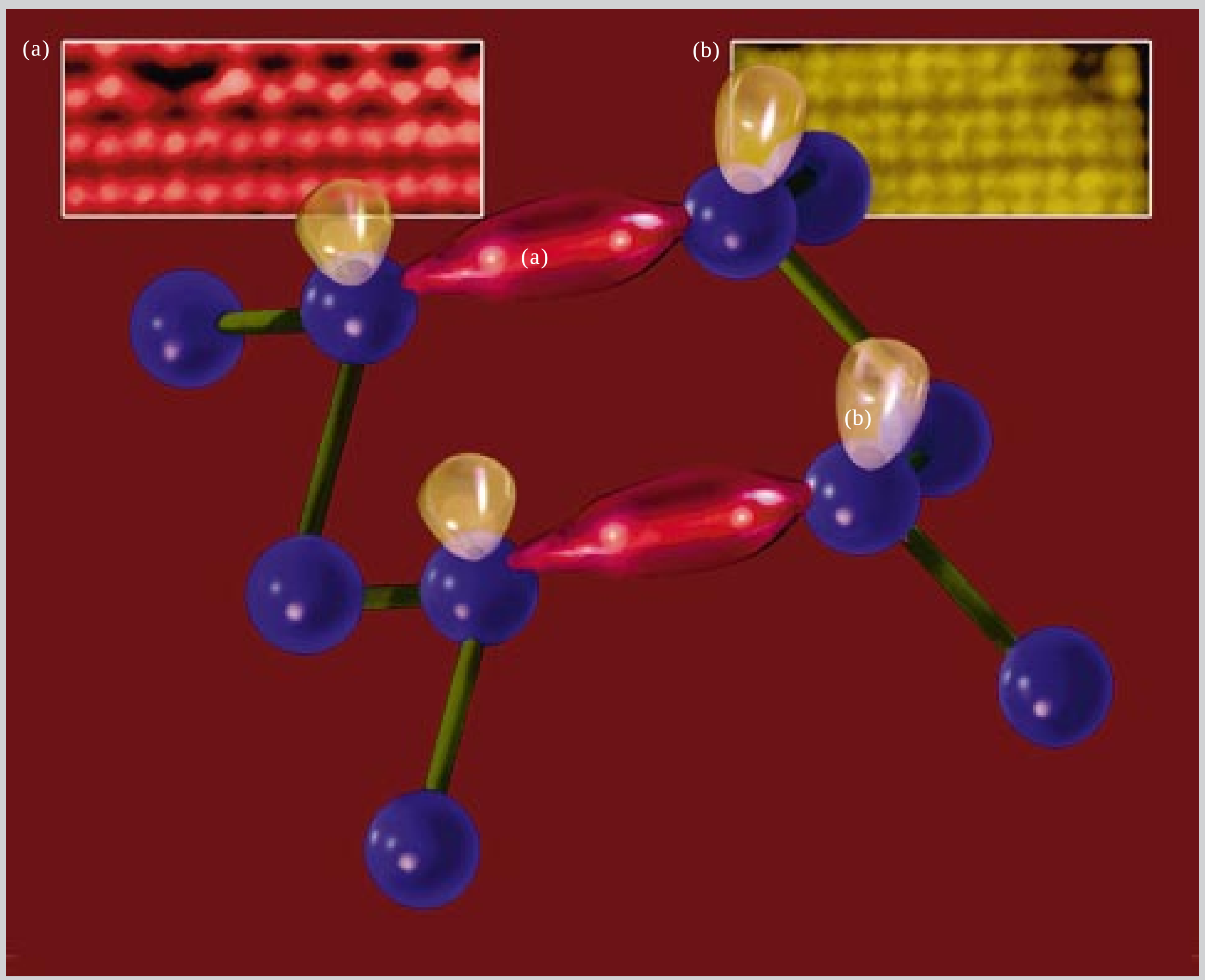
Regimes of Silicide Film Growth

When we use STM to examine these films, we find several regimes of silicide film growth. When molybdenum is

Imaging Surface Electronic Structure with STM

Because the trajectory executed by an STM tip is determined by the overlap of the electronic-state density of the tip with the local electronic-state density of the surface, the STM can be used to extract chemical information associated with a particular surface structure. On the Si(l00) surface, for example, dimerization results in a concentration of valence electron density between dimerized atoms (bonding orbitals) and a depletion of valence electron density in "anti-bonding" orbitals, of which there is one for each surface atom. In the model below, which presents the bonding geometry of a pair of dimers on the surface of Si (100), the bonding orbitals are represented in red, and the antibonding orbitals in gold.

If the STM is operated with a positive tip-to-sample junction, so that electrons must tunnel from the surface to the tip, the concentration of surface valence electron density within dimers causes the STM image to display rows of dimers, as in image (a) below. The individual dimers, displayed in red in image (a) correspond to the dimer bonds shown in red in the model. If the polarity is reversed, and electrons tunnel from the tip to the antibonding orbitals of the surface, then the resulting image (b) will enhance individual atoms. Each gold spot in image (b) then corresponds to one antibonding orbital, which in turn is associated with a single surface atom, as shown in the model.

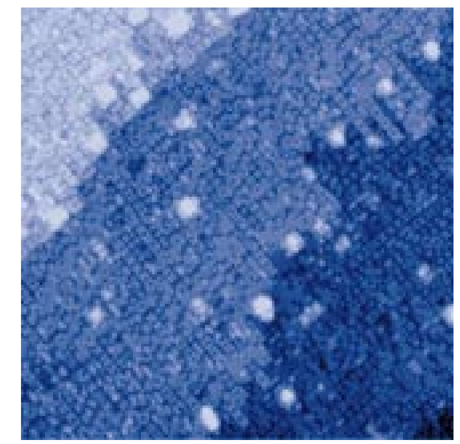


deposited on Si(100) at 475°C, a novel ordering of atoms occurs only within the outermost layer of the surface (Figures 3 and 4). Because this ordering cannot be detected by conventional x-ray crystallography and is not readily detectable by electron diffraction, the resulting surface previously was thought to be amorphous. With STM, it is now possible to identify the presence and locally ordered character of this new interfacial material.

At higher temperatures (between 650 and 750°C) in this process, some of the material nucleates into the hexagonal phase of disilicide $MoSi_2$ (Figure 5). This nucleation acts as a precursor for disilicide grains that grow when additional molybdenum is deposited on the surface.

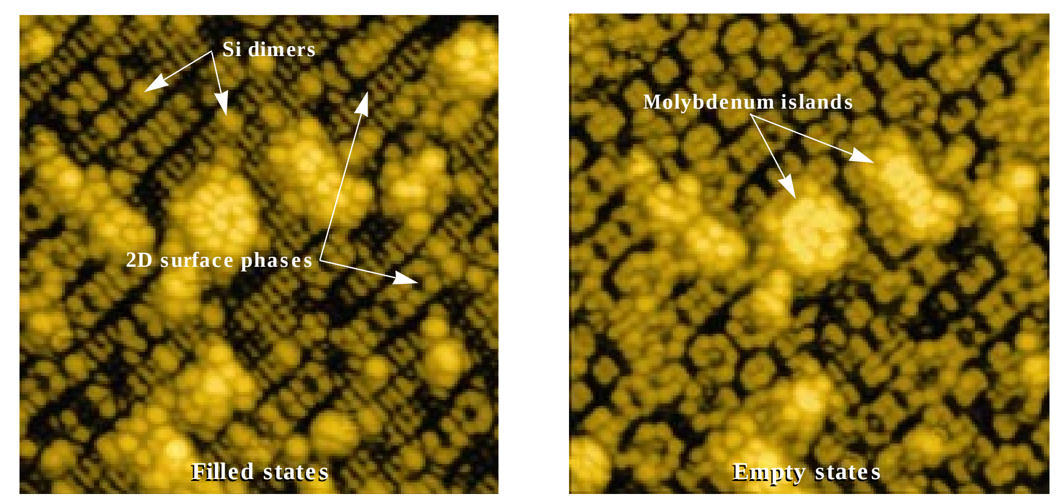
The third regime of disilicide growth occurs above 750°C. When molybdenum is deposited at 770°C, tetragonal $MoSi_2$ is formed. Figure 6, an STM image of the resulting surface, displays plateaus with large, flat terraces. Despite the variety of atomic arrangements observed in this image, each superstructure suggests a simple relationship to the periodicity (ordered, repeated atomic arrangement) of a specific face of tetragonal $MoSi_2$. The crystal face visible in the image then specifies the orientation of growth of the specific grain, which is preferentially oriented with respect to the silicon substrate.

For example, the sets of small circles in the three diagrams on the right-hand side of Figure 6 represent the atomic arrangement of the [001] planes of tetragonal $MoSi_2$. The large, shaded circles represent atomic sites in a superstructure that would correspond to the periodicity observed in the regions of the STM image. In the diagram on the left-hand side, the small, white circles represent silicon atoms in [100] planes, and the small, dark circles represent molybdenum atoms in those planes. The large shaded circles then constitute a superstructure that would correspond to the periodicity in the indicated region of the image rotated approximately 37 deg with respect to the neighboring regions. Such rotation would be required to achieve alignment between a disilicide crystallite growing



500 Å

Figure 3. A 500-Å atomic-resolution STM image of Si(100) following deposition of one-half monolayer of molybdenum at 475°C. The surface atoms form ordered arrangements over short ranges.



120 Å 120 Å

Figure 4. Filled- and empty-state STM images showing a 120-Å detail of the region shown in Figure 3. Each spot corresponds to a single surface atom. Various atomic arrangements are indicated with arrows.

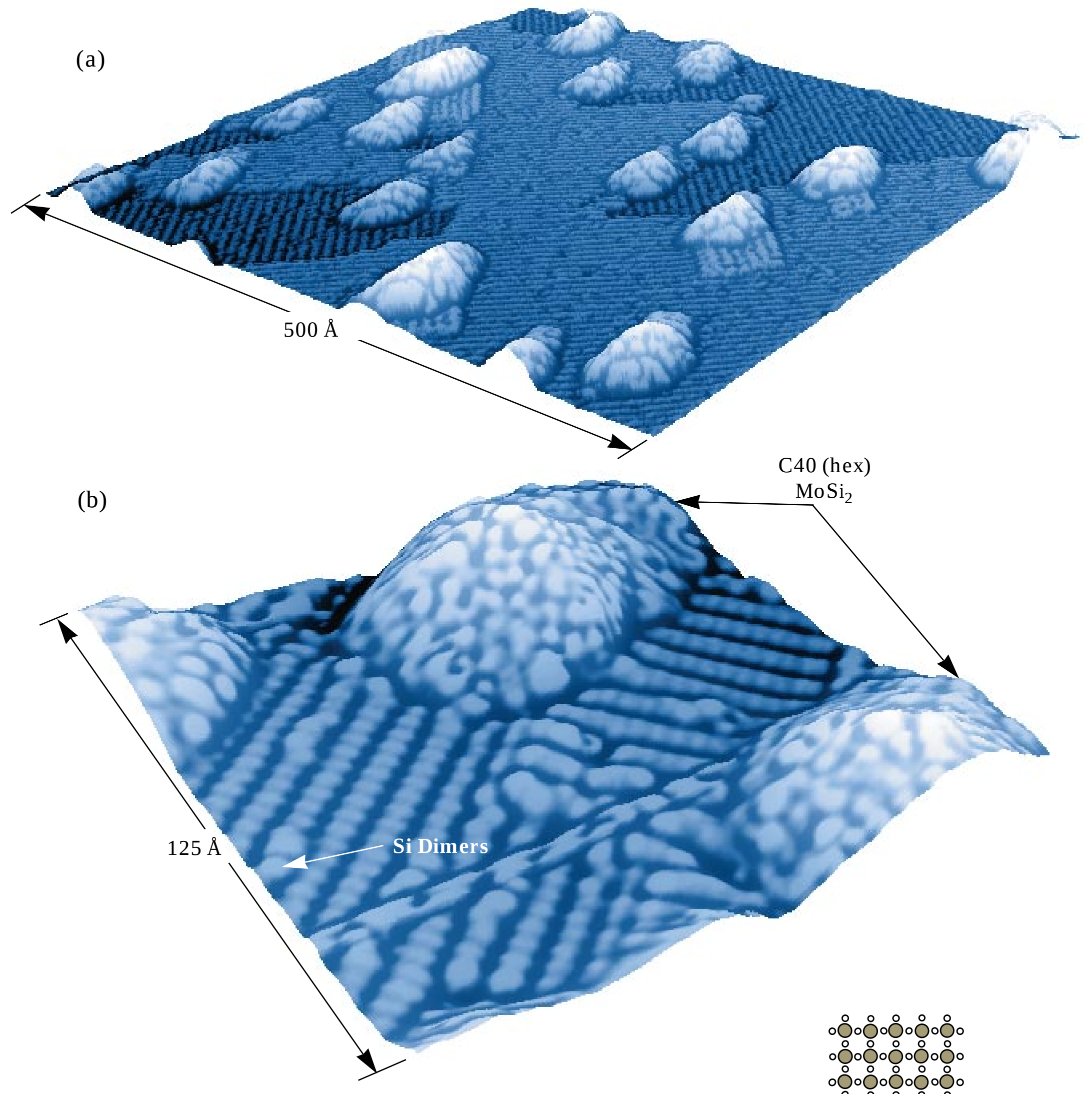


Figure 5. (a) A 500-Å STM image of Si(100) following deposition of one monolayer of molybdenum at room temperature and annealing at 640°C. (b) 125-Å detail showing individual silicon dimers and silicide islands.

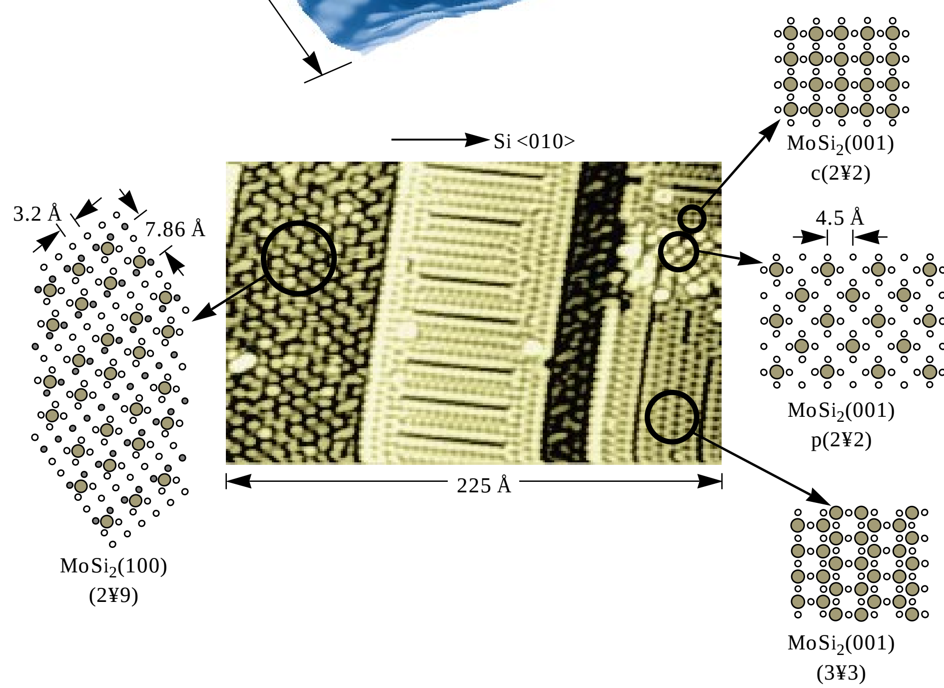


Figure 6. A 225-Å STM image of the surface resulting from the deposition of four monolayers of molybdenum on Si(100) at 770°C. The spacings between the atoms are indicated in the diagram.

along its <100> axis and one growing along its <001> axis. Both orientations of tetragonal $MoSi_2$ relative to the Si(100) substrate are consistent with those reported previously for thicker disilicide films. Neither the existence of these superstructures nor their relative prevalence was accessible from measurements used in previous analyses of the molybdenum/silicon system.

By associating specific microstructures with the temperatures at which they are processed, we are now equipped to determine the best procedure for synthesizing thin films that have the microstructures necessary for particular applications. For example, the temperature stability of multilayers used in x-ray mirrors is known to be related strongly to the microstructure of the interfaces between individual molybdenum and silicon layers.[6] The deliberate promotion during fabrication of one or another of the regimes of Mo/Si interfacial structure that we have identified above may therefore lead to multilayers with internal structure engineered for enhanced thermal stability.

With the advanced capabilities of STM, the Laboratory can evaluate how processing parameters affect the atomic structures of interfaces, identify surface defects that have a critical influence on film growth, and control their occurrence, which will lead to improved new materials with better performance characteristics.

Key Words: atomic ordering, disilicide, interface, molybdenum/silicon, nanoengineer, scanning tunneling microscopy, silicide, surface physics, thin film.

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About the Scientist

PETER BEDROSSIAN came to Livermore in 1992, when he joined the Chemistry and Materials Science Department as a Staff Physicist. He also works with the Advanced Microtechnology Program. In his short career here, he was a collaborator with a group at Sandia National Laboratories, Albuquerque, that received the 1994 Materials Science Award for Sustained Outstanding Research in Metallurgy and Ceramics from the U.S. Department of Energy. He has published 20 papers in the field of atomic-scale physics, including a number of articles in scanning tunneling microscopy.

Bedrossian received his A.B., A.M., and Ph.D. in Physics from Harvard University in 1985, 1987, and 1989, respectively. Prior to coming to Livermore, he worked at Sandia National Laboratories, Albuquerque, in the Surface Science Division from 1991 to 1992 and was a Humboldt Research Fellow at Forschungszentrum Jülich, Germany, in 1993.

Risk Assessments:

From Reactor Safety to Health Care

In LLNL risk-assessment experience, the most useful aspects of risk assessment are not exclusively the risk numbers that are generated, but also the insight gained from a systematic and methodical consideration of what can go wrong with a system.

OUR expertise in risk assessment has evolved over 20 years of experience. Lawrence Livermore National Laboratory's Fission Energy and Systems Safety Program (FESSP) first helped the Nuclear Regulatory Commission (NRC) to set up guidelines for safely siting and building nuclear power reactors. Today's challenge is to meet increasing needs to evaluate the safety risks of diverse, engineered systems.

Risk-analysis techniques have been used by both government and industry to study and assess the safety, reliability, and effectiveness of various products, processes, and facilities. We performed original probabilistic risk analyses in three important areas: seismic safety in U.S. nuclear power plants, regulations in transporting spent nuclear reactor fuel, and, most recently, human-initiated risk in using a nuclear medical device. These assessments have evolved into the development of new methods and techniques, subsequently affecting regulatory developments and broadening the range of applications and usefulness for risk analysis.

Health Versus Engineering Risk Assessments

In many cases, a risk assessment focuses on the health effects that occur when toxic chemicals are released from a product, process, or facility and enter the environment. This type of risk assessment is often referred to as a health risk assessment and is commonly undertaken by agencies of the federal government that deal with public health and safety, e.g., the Environmental Protection Agency, the Food and Drug Administration, the Consumer Product Safety Commission, and the Occupational Safety and Health Administration.

Other times, a risk assessment focuses on the health effects that can occur when an "engineered" system fails, because of a natural or human-initiated event or when the protective barrier between the environment and that system fails (Figure 1). Known as engineering risk assessments, they are commonly carried out by agencies of the federal government that make safety, health, or design decisions about risk-posing facilities or equipment. Examples of agencies that use engineering risk assessments are

- Department of Energy, in evaluating the radiological and chemical risks from various types of nuclear and non-nuclear facilities.
- Department of the Interior, in analyzing dam safety, assessing damage from ecological disasters, and helping to predict natural hazards, such as earthquakes, floods, or volcanoes. Much of this risk assessment work is directed toward improving the probability distributions that describe the recurrence of these natural hazards and their possible intensity.
- Federal Aviation Administration, in analyzing potential collision scenarios, such as the simultaneous approach of two aircraft on closely spaced, parallel runways in inclement weather.
- National Aeronautics and Space Administration, in assessing the possibility of shuttle accidents that might result in the release of radioactive material from radioactive power sources.
- Nuclear Regulatory Commission, in analyzing risks of low-level radioactive waste disposal, evaluating performance of high-level waste repositories, and evaluating risks associated with nuclear power plant accidents.

The Assessment Process

Although the process used to assess risks from engineered systems varies with each user and application, it usually retains five common elements (Figure 2):

- A description of the system's hardware components, operating environment, and staff operators.
- A hazard identification analysis to determine the events or conditions that might lead to accidents or failures.
- An analysis to estimate the frequency of events that must occur before health impacts could occur.
- An analysis to determine the health effects, i.e., the consequences of these events to workers and the public.
- A procedure to quantify assessed risks, including the uncertainties inherent in any risk evaluation.

In 1983, the National Academy of Sciences published a document that standardized the process for health risk assessment. The book, *Risk Assessment in the Federal Government: Managing the Process,*[1] is also known informally as the "Red Book."

The Red Book breaks the risk assessment process into four basic elements:

- A hazards identification analysis to determine whether a particular chemical is or is not causally linked to a particular health effect.
- An exposure assessment to determine the extent of human exposure before or after the application of regulatory controls.
- A dose-response assessment to determine the relation between the magnitude of exposure to a chemical

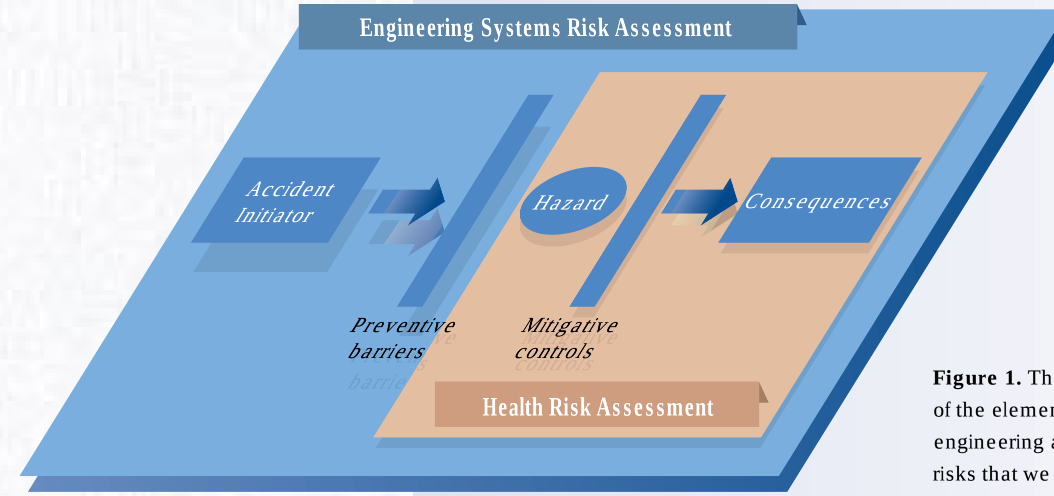
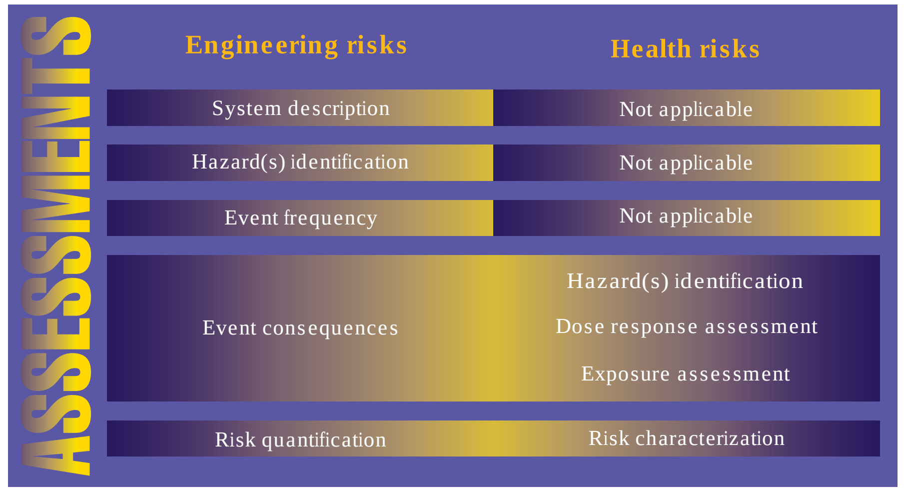


Figure 1. The interplay of the elements of engineering and health risks that we evaluate.

Figure 2. Some components of engineering systems risk assessments overlap those for health risk assessments.



and the probability of occurrence of the health effect in question.

• A risk characterization procedure to describe the nature and magnitude of human risk, including any attendant uncertainty.

If we compare these health risk assessment elements to the five basic elements of engineering risk assessment, we find both similarities and differences between the two processes. In an engineering risk assessment, the event consequence step contains the first three steps described in the Red Book (Figure 2). In NRC studies that analyze the impact from a release of radioactive material, this consequence would be the dispersion of material in the environment; the uptake of the material via inhalation, ingestion, or other exposure pathways; and the response of various body organs to such exposures. The results would lead to an estimate of the probability of cancer incidence or fatality, given that the radioactive release had occurred.

Perhaps the most significant difference between the two processes is the treatment of event frequencies. In an engineering risk assessment, the analyst considers both the frequency of an event (e.g., a large earthquake occurring near a nuclear power plant) and the probabilities of different failures within the engineered system. Different combinations of failures can lead to health threats of different severity. For example, an earthquake could produce a variety of damage in a nuclear power plant, including no damage at all. These damage states could, in turn, lead to a variety of potential radioactive releases, or no release at all. Thus, a single initial event can lead to a variety of possible health effects, each with its own probability.

On the other hand, in a health risk assessment, the analyst deals primarily with situations involving chronic releases to the environment with a release probability of 1, that is, the assumption that such a release will absolutely occur. This type of assessment would propose to restrict or eliminate the material's presence rather than mitigate with engineering controls or boundaries.

The differences between engineered-system risk assessment and health risk assessment thus have a significant impact on risk-management strategies. Although eliminating hazards is an effective strategy, it is not always practical in an industrialized economy. Engineering risk assessment supports the management of risk through design, maintenance, and administrative controls. Reducing the possibility that accident initiators and hazards can cause consequences—through effective and reliable engineered barriers and mitigative controls—provides a means of managing risks in industrial activity while protecting the environment, safety, and health of the public.

Another important difference between the two processes has to do with consequence measures, or endpoints, of risk assessment. Health risk assessment is specific to exposures from toxic chemicals and the associated dose response; hence, the ultimate endpoint can be cancer fatality. In engineering risk assessment, the endpoint varies. Common endpoints include worker health and safety, loss of a facility or piece of equipment (for example, the crash of an airplane and the associated, implicit health effects), immediate loss of life (one of the results of a large earthquake), or long-term loss of life from cancer (one of the results of a nuclear power plant accident). In addition to these consequences, engineering risk assessment can have other nonhealth-related endpoints. For example, the endpoint of a Department of the Interior risk assessment study on dam failure involved the economic impact that failure would have on the surrounding community.

Our Focus: Engineering Risk Assessment

Depending on its application, an engineering risk-assessment study can fall into one of five classes: it can be a conceptual design evaluation, a detailed design study, a facility operations study, a management support study, or a policy and standards development study. Table 1 offers examples of the applications or activities appropriate to each class. Conceptual design evaluations and detailed design studies tend to focus on equipment or one facility at a time; facility operations, management support, and policy standards and development studies can focus on a single facility or on multiple facilities and activities.

The FESSP specializes in integrating advanced analytic methods with an understanding of nuclear technologies, economics, and policy-making. Over the last 20 years, we have performed a number of original risk-assessment studies to support regulatory developments at the NRC. We concentrate on safety issues relating to engineered systems that either use or contain nuclear material, as shown in the following four cases:

• An analysis to develop seismic criteria for the siting and design of nuclear power plants.

• A risk analysis of reactor coolant piping systems to establish new piping design objectives and increase nuclear power plant safety.

• A study of risks involved in the transport of spent reactor fuel to determine the level of safety provided during transport and the adequacy of existing transport regulations for such material.

• The development of an approach to identify human-initiated risks in the use of nuclear medical devices such as the Gamma Knife.[2]

Depending on the nature of the problem, the detailed methods used in each study vary in that they may include any or all of the basic elements of the engineering risk-assessment process. However, each study is similar in that it constitutes a rational and systematic approach to obtaining information that can be used to increase safety, formulate policy, develop standards, omit costly duplications, or implement regulatory guidelines.

Our evolving experience base thus provides the government with recommendations of risk-based regulations and prioritizations for resource allocations. It shows where regulatory reform can help the

Table 1. Classification of engineering risk assessment by application or activity.

Type of engineering risk assessment	Application or activity
Conceptual design evaluations	• Determine the viability of a particular site for a particular facility. • Analyze and compare competing technologies or processes. • Evaluate the risks of emerging technologies.
Detailed design studies	• Identify risk-dominant scenarios to provide guidance for refinements in the design of a system or facility. • Analyze and compare the reliability or availability of system/component options. • Provide specifications to design components, systems, or structures that will have high reliability and protection against severe natural phenomena. • Analyze and improve a facility's training programs, operator–equipment interfaces, and operating procedures. • Determine optimum safety limits, equipment outage times, and testing frequencies to minimize risk. • Analyze acceptable risk to document the importance of risk-based design features and systems interactions data.
Facility operations studies	• Carry out a risk-based analysis of operating events. • Design and implement risk-based trends and patterns. • Improve system availability. • Enhance component inspection, testing, monitoring, and maintenance based on component failure analysis. • Evaluate and prioritize safety issues. • Evaluate, select, and schedule modification. • Assess continued operations. • Enhance safety, emergency, and accident management information and training.
Management support studies	• Provide risk-based perspectives for decision-making. • Provide information for allocating resources (staff, budgets) and identifying research needs. • Measure safety performance. • Perform risk-based quality assurance and audits.
Policy/standards development studies	• Assess and develop rules, standards, and safety criteria. • Develop safety measures, goals, and criteria. • Assure coordination and consistency of safety goals and criteria.

government—and the country—work better and safer for less.

Case 1: Seismic Criteria for Siting Nuclear Power Plants

Since the early 1970s, the Laboratory has worked with the NRC to establish seismic criteria for regulating the siting of nuclear power plants. Most of these criteria are deterministic in that they are based on the determined size and location of the most credible seismic event, not on its frequency of occurrence or the possible consequences. In areas where very large earthquakes have occurred (such as New Madrid, Missouri, or Charleston, South Carolina) or cannot be excluded from occurring, even if the likelihood of occurrence is very small, the application of siting regulations based on these criteria could lead to very conservative design criteria and prohibitive costs.

To help the NRC evaluate the effect of such siting regulations, we proposed to assess the seismic hazard by using a probabilistic methodology—that is, we weighted all the possible earthquakes that could affect a site by their likelihood of occurrence. By coupling this methodology with a newly developed systems analysis concept, we systematically analyzed the series of causative events and the behavior of all structures, systems, and components in the plant. We then identified the failure modes and quantified their consequences. The total risk was obtained by considering the entire spectrum of earthquakes and all possible modes of failure and integrating their calculated consequences (Figure 3).

Sponsored by the NRC, this first U.S. seismic probabilistic risk assessment for nuclear power plants from 1978 to 1985 cost $18 million. The same methodology was then used by the nuclear industry to assess 35 nuclear power plant sites. The majority of seismic probabilistic risk-assessment knowledge existing in the technical community today was gained through this massive exercise.

Our methodology is now widely used by the NRC and other public utilities to evaluate and compare, on a relative scale, the risks associated with existing nuclear power plants. In many cases, its use has led to retrofitting, reinforcement, and redesign of components or systems to achieve comparable levels of risk across the entire population of plants.

Currently, we are helping the NRC to overhaul the seismic siting criteria for new nuclear power plants. Our experience base has been used to help develop proposed risk-based regulations now under public review. Previous regulations were based on methodologies that rely on single deterministic models. Often such models pit one group of experts against another group, creating time delays and thus protracting the plant licensing process. The proposed changes to regulations are based on a methodology that provides a framework for assessing all information and makes maximum use of existing data and factors from all possible modeling and scientific alternatives. As such, the changes should help streamline the plant licensing process.

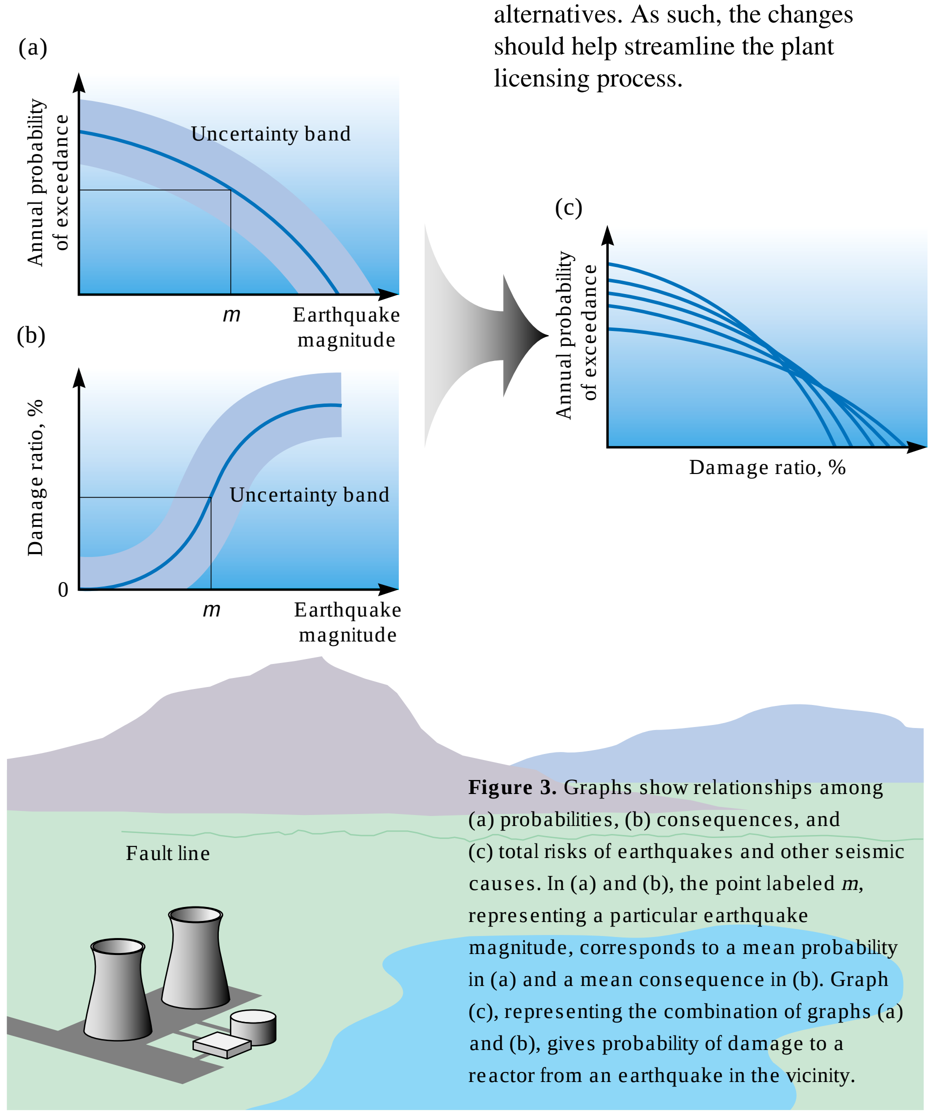


Figure 3. Graphs show relationships among (a) probabilities, (b) consequences, and (c) total risks of earthquakes and other seismic causes. In (a) and (b), the point labeled *m*, representing a particular earthquake magnitude, corresponds to a mean probability in (a) and a mean consequence in (b). Graph (c), representing the combination of graphs (a) and (b), gives probability of damage to a reactor from an earthquake in the vicinity.

Case 2: Safety of Reactor Coolant Piping

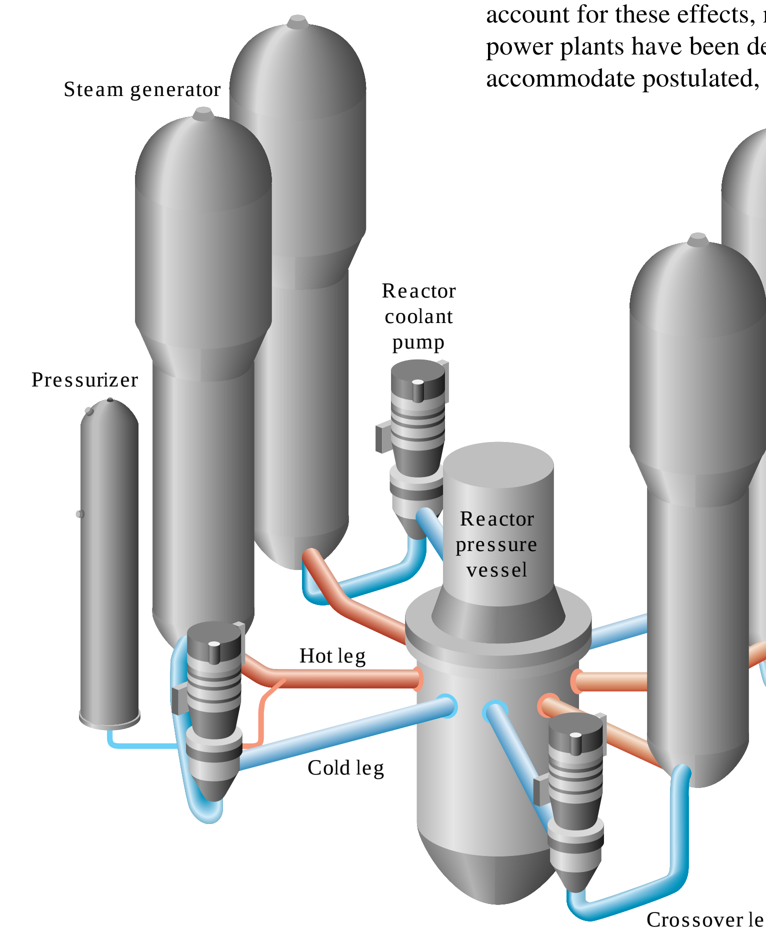
This safety assessment was one of the first Laboratory studies in which risk-assessment techniques resulted in regulatory change. It is also a classic example of a substitution risk, that is, substituting a change in risk for a savings in dollars.

The *Code of Federal Regulations*[3] requires that structures, systems, and components important to the safety of nuclear power plants be designed to withstand the effects of naturally occurring hazards as well as the effects of normal and accident conditions. Design criteria require that safety-related structures, systems, and components of nuclear power plants be designed to withstand the effects of a large loss-of-coolant accident. To account for these effects, nuclear power plants have been designed to accommodate postulated, double-ended, "guillotine" breaks in their high-energy piping systems, particularly the massive ones about a meter in diameter that circulate primary reactor coolant (see Figure 4a).

The difficulty—and cost—of designing a nuclear power plant for postulated pipe breaks was exacerbated by a related requirement that the hydrodynamic loads be combined with the vibratory loads that result from a "safe shutdown earthquake," the maximum design-basis earthquake for a nuclear power plant. In effect, this requirement presumed that an earthquake could cause pipe breaks in all high-energy piping systems. This requirement was also problematic because the design objectives for safe piping systems under normal conditions contradicted those for safe piping systems under earthquake conditions.

During normal operation, piping systems must be flexible enough to expand to relieve the thermal stresses that can drive cracks through their walls and cause leaks or breaks. However, during a large earthquake (which is most likely a once-in-a-plant-lifetime occurrence), stiff piping is needed to assure that seismically induced breaks

(a) A reactor coolant piping system



(b) Failure probability

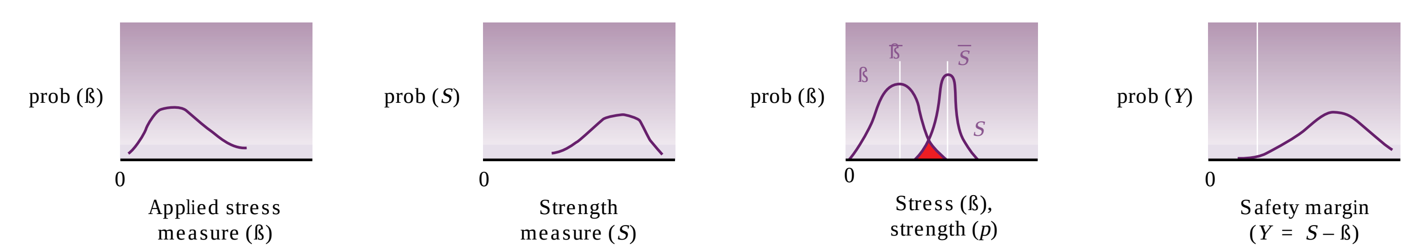


Figure 4. (a) LLNL developed standards and proposed regulations concerning the high-energy piping systems that circulate primary reactor coolant. (b) Probabilistic approach for assessing component adequacy for postulated load conditions in piping. In this approach, failure is possible only in the region shaded red.

do not occur. Designers have met these cross purposes by using “pipe snubbers,” elaborate mechanical and/or hydraulic devices that allow pipes to move during normal operation but anchor them rigidly when they are subjected to rapid (i.e., seismic) loads. Pipe snubbers not only require periodic testing and maintenance—in areas of high radiation and difficult access—but have proved unreliable. Many have been found to lose their earthquake-resisting function; others have been found to restrict normal thermal expansion and seriously increase pipe stresses. (In the latter mode, then, these safety devices can actually increase the likelihood of pipe failure.)

For years, nuclear plant designers have contended that the likelihood of seismically induced breaks is low enough to be considered negligible. They believed that protective measures such as pipe whip restraints and jet impingement barriers may actually decrease the reliability of piping systems. In the early 1980s, the nuclear industry sought to exempt itself from the NRC piping safety regulations by doing extensive research in deterministic fracture mechanics so that it could argue the merits of a “leak-before-break” concept. That is, because of the very tough materials used in nuclear piping, even large cracks through walls would remain stable and not result in a double-ended guillotine break. The NRC sought additional technical information to respond to the exemption request.

The FESSP engineers, in an independent confirmatory research effort funded by the NRC Office of Nuclear Regulatory Research, developed and applied risk-assessment techniques (Figure 4b) to estimate the likelihood of a double-ended guillotine break in the coolant loop piping of a pressurized water reactor (PWR). This effort consisted of the “Flexible vs Rigid Piping Program,” “Piping Reliability Program,” and “Load Combination Program” carried out between 1981 and 1985 at a cost of $3.5 million.

The results of this analysis indicated that the probability of this kind of break in a PWR’s coolant loop piping is low enough under all plant conditions, including earthquakes, to justify eliminating it as a basis for plant design. Our analysis also showed that the probability of a pipe break being caused by an earthquake is significantly less, by a factor of 10 to 100, than the probability of a pipe break being caused by thermal stress. The results of a companion probabilistic analysis of stiff versus flexible piping supported the opinion that inadvertent stiffness (resulting, for example, from failed pipe snubbers) can indeed reduce nuclear power plant safety.

On the basis of these technical results, we recommended that the NRC eliminate the double-ended guillotine break requirement in the reactor coolant loop of PWR designs. After an exhaustive peer review of the results by technical experts, the provisions of General Design Criterion 4 were modified by excluding from the design basis any dynamic effects associated with loss-of-coolant accidents. Our technical analyses made it possible to apply the new exclusion rule to the main reactor coolant loop piping in all U.S. PWR plants.

The rule change also indicated the removal of pipe snubbers—a decision that had two major effects. First, it reduced the amount of time that maintenance and inspection personnel had to spend in high radiation areas, thus reducing their exposure to radiation. Second, the nuclear power industry no longer had to design, fabricate, install, and maintain the costly snubber equipment. Industry spokespersons say that the rule change has resulted in savings of tens of millions of dollars for each nuclear power plant.

Case 3: Assessments for Transporting Spent Nuclear Fuel

Tens of thousands of spent nuclear fuel assemblies from U.S. nuclear power plants are currently being stored at the plants. In the near future, these spent fuel assemblies will be placed in a federal repository for permanent storage.

From 1985 to 1987, we performed a transportation model study for the NRC to determine the level of safety provided when spent reactor fuel is transported to a nuclear waste repository. During transport, the protective casks carrying the fuel could be exposed to highway or railway accidents. Our task was to evaluate and document what might happen to the casks under severe conditions and to assess how effectively the current federal transport regulations would protect the public.

This assessment represented a departure in risk-assessment techniques from reactor safety studies. The nuclear power plant probabilistic risk assessment addresses stationary facilities, with system functions and potential faults fairly well understood. In this assessment, a first in transportation regulations, we studied scenarios having nuclear material moving

through populations, with various potential highway and rail accidents.

Spent fuel shipments, now occurring at a very low rate, are regulated by both the Department of Transportation (DOT) and the NRC. The NRC evaluates and certifies the design of the shipping casks used to transport spent fuel, and DOT regulates vehicles and drivers. Current NRC regulations require that shipping casks meet certain performance standards. For example, under normal operating conditions and hypothetical accident conditions, a cask must limit releases of radioactive material and minimize external radiation levels, and it must assure that the spent fuel will remain subcritical (not undergo a self-sustaining nuclear chain reaction).

The study evaluated the possible mechanical and/or thermal forces generated by actual truck and railroad accidents. The magnitudes of forces from actual accidents were compared with forces attributed to the hypothetical accident conditions defined in the NRC and DOT regulations (Figure 5). The frequency of accidents that can produce defined levels of thermal or mechanical force was also developed. With this information, the study results showed that for certain broad classes of accidents, spent fuel casks provide essentially complete protection against radiological hazards. For extremely severe accidents imposing forces on the cask greater than those implied by the hypothetical accident conditions, we made calculations of the likelihood and magnitude of any radiological hazard.

The study also contained an evaluation of the radiological risk from accidents during transport. Risk represents the summation of the products of the magnitude and likelihood of all accident outcomes. The purpose for making the risk calculations was to compare the resulting values with those previously used by the NRC in judging the adequacy of its regulations. We confirmed the adequacy of existing regulations. Our methods subsequently have become the basis for other transportation risk studies required by DOE/Defense Programs and DOE/Office of Civilian Radioactive Waste Management.

Case 4: Identifying Risks of Using Nuclear Medical Devices

Our experience with analyzing risks of radiation-emitting systems has led to performing other radiation-based analyses. In one of these cases, involving a medical application, we found it necessary to develop new techniques to evaluate the potential risks of a relatively new device for which operators have limited operating experience and processes have substantial human-factor considerations.

As part of its public health and safety charge, the NRC is responsible for regulating radiation from nuclear byproduct material. Current NRC regulations address procedures for conventional cobalt-60 teletherapy devices, but do not necessarily address appropriate or comparable procedures for the Gamma Knife (Figure 6), a commercially available external-beam radiation device. It is used to locate and surgically treat inaccessible lesions in the brain while sparing healthy tissue along some 200 radiation entry paths.

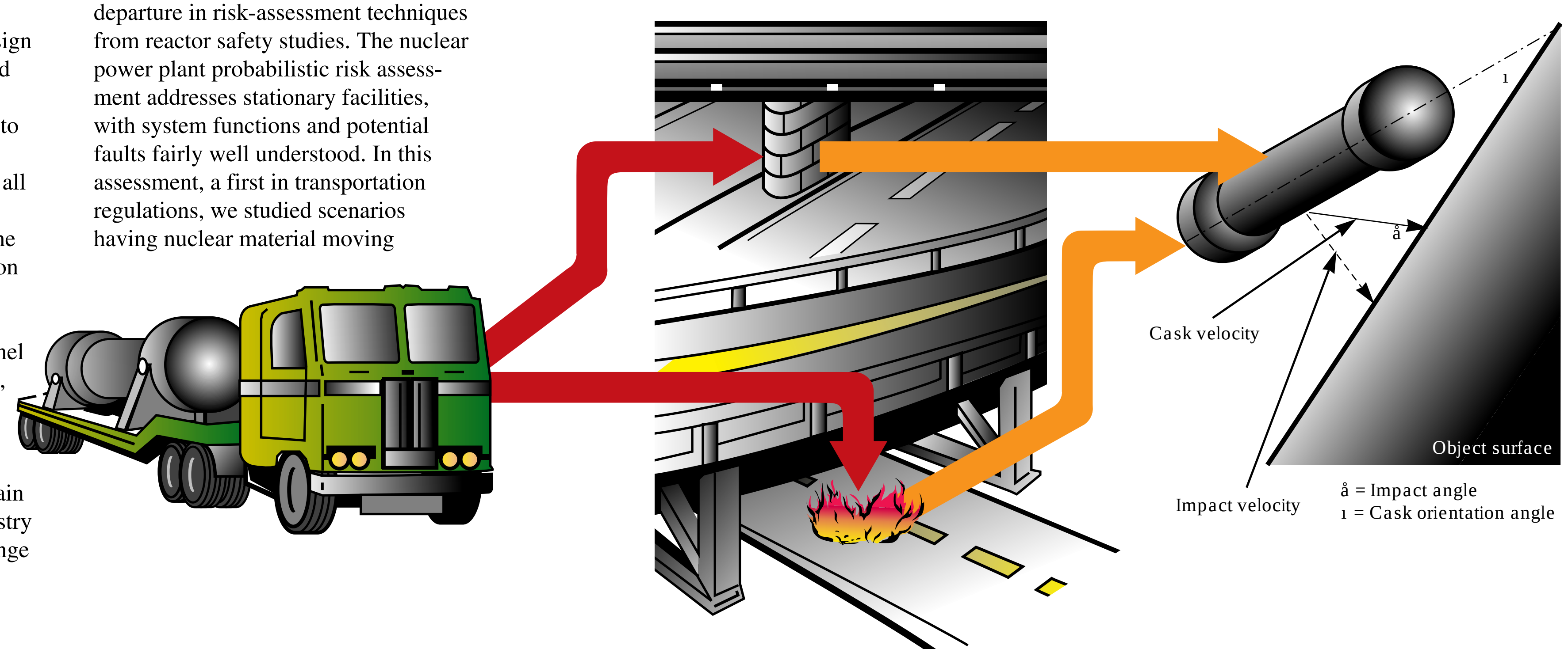


Figure 5. Comparisons were made of forces from actual transportation accidents and hypothetical conditions for a risk assessment of transporting spent nuclear fuel. Damage to the cask depends on the velocity of the cask and its orientation when it impacts a hard surface.

Reports received by the NRC pointed to some cases of misadministration in conventional teletherapy that have resulted from equipment malfunctions or human errors in treatment planning, dose calculations, and measurements. It was reasonable to project that comparable events may occur with the Gamma Knife.

The NRC therefore asked us to perform a preliminary risk analysis of the use of the Gamma Knife. Our review of cases of misadministrations and abnormal occurrences for conventional teletherapy indicated that the assessment of the risks of such an external beam therapy system should be balanced between equipment failures and human mistakes, if not skewed toward the human errors.

The Gamma Knife is used to deliver gamma radiation from cobalt-60 to precisely defined, intracranial targets. Its relatively simple hardware system requires significant human control, but because the instrument is relatively new, very little operating failure data exists for it. Most operational information resides in the, as yet, limited and little-documented experience base of the manufacturer and operators. FESSP was asked to identify the high-risk, human-initiated actions and failure modes that are most likely to occur and to evaluate their relative importance.

To do that, we adopted an approach that relied on empirical evidence, observations, and expert experience. In this approach, an analysis of the Gamma Knife treatment tasks provided a systematic framework that could adequately account for and describe activities and equipment that could lead to undesirable events or consequences. We relied on experts' estimates of likelihood, consequence, and risk for the primary tasks, and compared them by means of relative risk rankings and risk profiles. These estimates aided the identification of the highest-risk or critical tasks, without requiring an absolute quantification of risk for each task.

We believe the approach may be best used to identify weaknesses in processes and to support the development of positive performance measures, rather than to predict the numerical risk associated with poor performance. Perhaps most effective in nuclear medical applications that are not highly structured, the approach could serve to produce reliable processes and procedures to prevent misadministrations that result from mistakes. We have yet to apply these principles and techniques elsewhere, but we expect them to be applicable where human-initiated actions are important. The lesson learned is that informative assessments can be made from a relative risk analysis; the approach is also inexpensive and practical.

When to Perform Risk Assessments

Risk assessment is an excellent risk-analysis tool in that it allows us to

- Systematically examine a broad set of design and operational features.
- Integrate the influence of system interactions and human–system interactions.
- Explicitly consider uncertainties in estimates.
- Consider and analyze competing risks—those of one system versus another, or of one set of modifications versus another.
- Measure the relative importance of systems, components, and other engineered elements to risk.
- Quantify the overall level of risk for a system.
- Identify relative risks versus cost tradeoffs in design and operational modifications.

However, risk assessment also has its limitations. It may sometimes exclude or not adequately quantify potentially important risk factors, such as very-low-frequency accident initiators, various failures derived from a common event, physical processes resulting from several low-frequency failures, or long-term health effects from potentially toxic materials. Furthermore, because a risk assessment often deals with low-frequency but high-consequence accident risks, there is considerable potential for its results to be misunderstood.

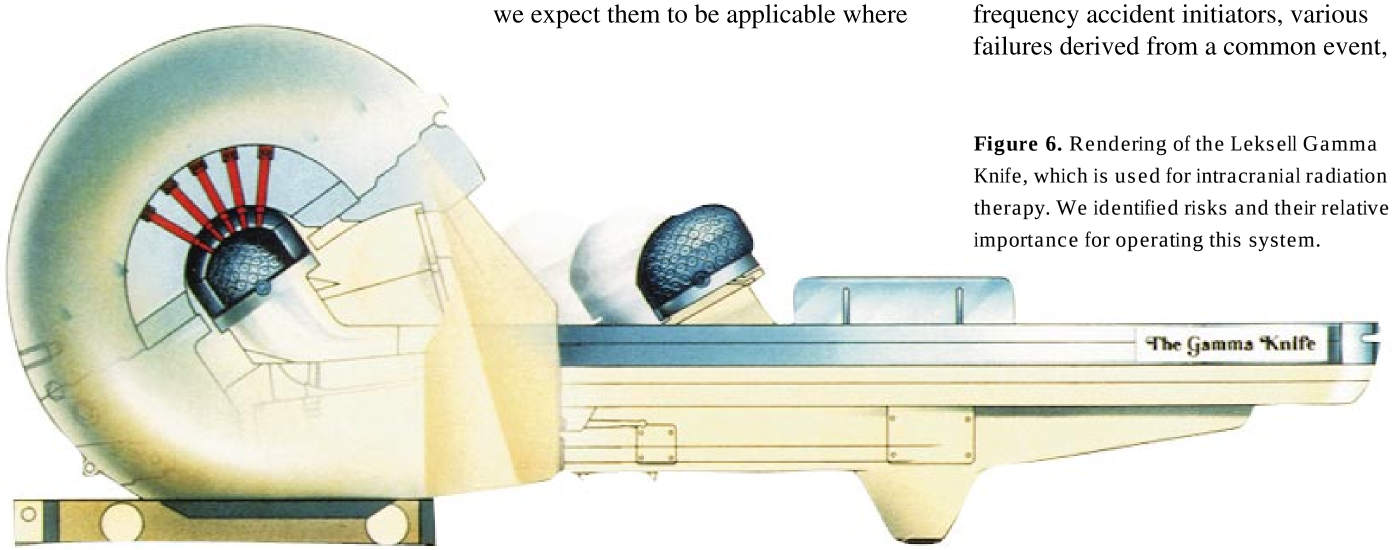


Figure 6. Rendering of the Leksell Gamma Knife, which is used for intracranial radiation therapy. We identified risks and their relative importance for operating this system.

In our experience, the most useful aspects of risk assessment are not exclusively the risk numbers that are generated; they are also the insight gained by a systematic and methodical consideration of what can go wrong with a system. A procedural analysis helps us to understand the likely vulnerabilities of the system, the threats they pose, and the measures that could be applied to mitigate or prevent them.

Risk assessment is a particularly powerful tool when there is only a limited set of alternatives for risk evaluation. "Real-world" managers, too, often have only limited resources to improve safety. Ultimately, the "best" choice will depend on the context of the manager's problem, as illustrated by our piping safety study.

We have found that it is important to do sensitivity, or "what-if," analyses to determine the relative importance of input to a risk assessment. Varied input allows us to (1) distinguish risks from variations in assumptions, modeling, or data; (2) identify where a lack of information is crucial; (3) determine which factors contribute the most to risk; and (4) investigate potential preventive or mitigative solutions that combine various risk-reduction measures. Because evaluations of alternatives or sensitivity analyses do not require absolute risk values, we can use relative risk estimates or risk rankings to compare risks. Relative risk estimates are adequate to compare alternative approaches to the same problem or to achieve comparable levels of risk across a population of similar systems. Thus, meaningful insights can be obtained by a risk assessment without depending on the accuracy of an "actual risk" value—such values are notoriously difficult to ascertain.

Uncertainty is a very important part of any risk assessment, particularly when there is an attempt to accurately quantify an actual risk. Uncertainty studies should be performed to evaluate the dependence of the assessment results on uncertainty values. Sources of uncertainty occur in models, methods, and data. Given the uncertainties inherent in any risk assessment, expert analysts may disagree over risk characterization values. Sometimes consensus is obtained by defaulting to the most conservative estimates. Such practices tend to "ratchet-up" prescriptive risk standards.

Because a risk analysis receives so much scrutiny, the risk assessment must be documented and understood. It is also extremely important to have the assessment reviewed by independent agents both internal and external to the organization performing the assessment.

Finally, the results of a risk assessment are only one of many inputs to a decision. Other factors—which may have nothing to do with technical risk per se—include cost considerations, compliance with rules and regulations, mission objectives, business operations, and public perceptions. The relationships among these factors can be complex, and the relative value of each is context dependent. Integrating these factors into the decision-making process is essential.

Key Words: engineering risk assessment; Fission Energy Systems Safety Program (FESSP), Nuclear Regulatory Commission (NRC); probabilistic, risk, risk assessment,

References

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2. Registered trademark of Elekta Instruments, Inc.
3. *Code of Federal Regulations,* Title 10, Part 50.

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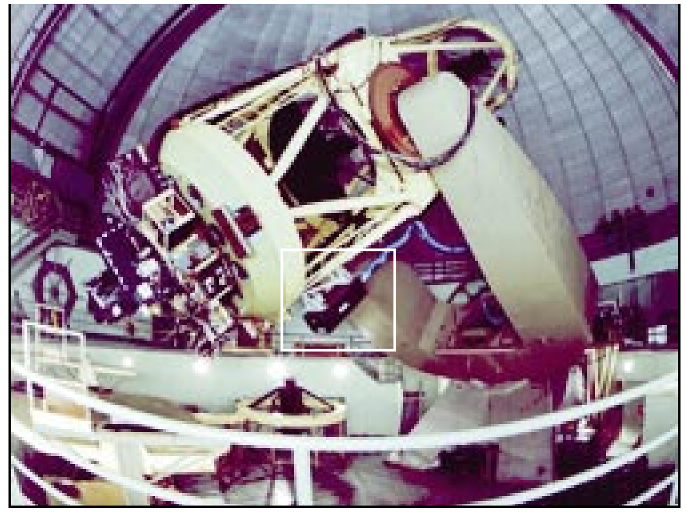
About the Engineer

ED JONES came to the Laboratory in 1991, when he joined the Fission Energy and Systems Safety Program. Since 1993, he has been the Deputy Associate Program Leader for Risk Assessment, System Engineering, and Human Performance. He has written ten papers on risk assessment since arriving in Livermore.

Jones received his B.S. degree in Engineering and Physics in 1975 from the University of California, Berkeley. He did graduate work in engineering and physics at Stanford University from 1975 to 1978 and doctoral research in physics from 1979 to 1981 at the University of Oxford. Before coming to LLNL, Jones worked at Eyring Research Institute from 1983 to 1987 and at BDM International, Inc., from 1987 to 1990; he was president of Jones and Associates from 1990 to 1991.

Crucial Steps Taken in Laser Guide Star System



EARTH-BOUND astronomers have long sought to diminish the effects of the atmosphere on their observations. Stars that appear as sharp pinpricks to the eye become smeared “blobs” by the time they are imaged by large ground-based telescopes.

At the University of California’s Lick Observatory on Mount Hamilton near San Jose, California, Laboratory researchers and their UC colleagues are installing a system on the 3-m Shane telescope that will correct these troublesome distortions. The system includes a dye laser that will create a “guide star” in the upper atmosphere and very sensitive adaptive optics that will measure and correct for atmospheric distortions. According to Scot Olivier, project scientist for the adaptive optics subsystem, the Shane is the first major astronomical telescope with such a laser system.

Other groups have been using adaptive optics systems with natural guide stars. However, it turns out that not just any star will do. It must be bright enough, that is, generate enough light to serve as a reference. When observing at visible wavelengths, astronomers using adaptive optics require a fifth-magnitude star, one that is just bright enough to be seen unaided. For near-infrared observations, only a tenth-magnitude star is needed, which is 100 times fainter.

The problem, Olivier noted, is that even though there may be hundreds of thousands or even a million stars bright enough to be guide stars, they only cover a small fraction of the sky. “Many times, there just isn’t a natural guide star in the area you want to observe,” he said. “This is the kind of situation where a telescope equipped with a laser guide star comes out ahead.” (See box.)

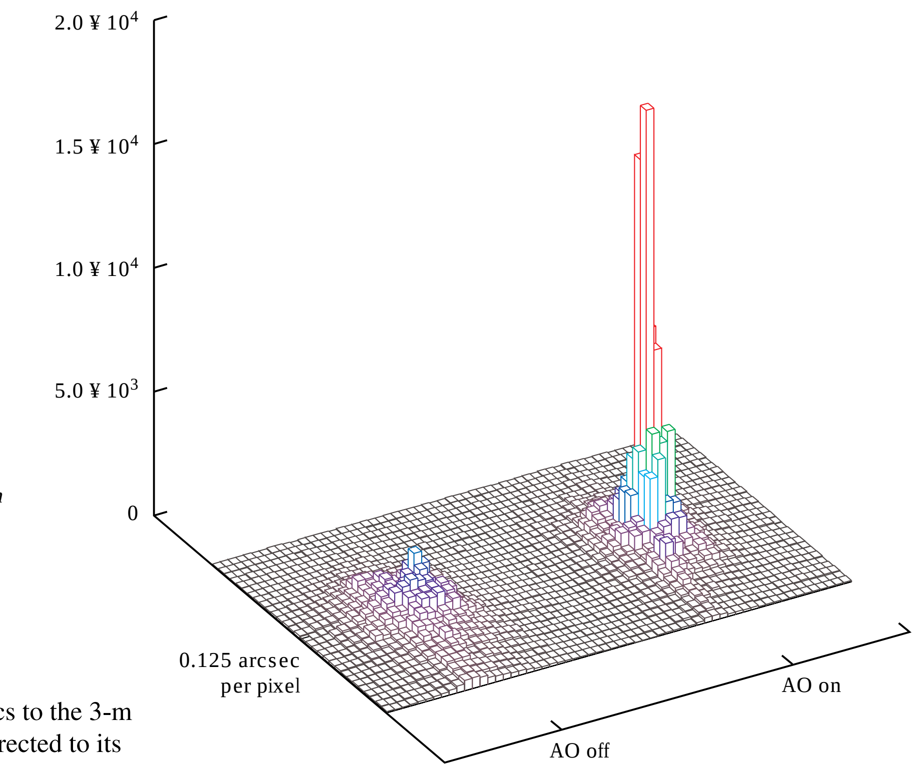
The guide star is created by a dye laser system, which is a small, closely related version of the system used by the Laboratory’s Atomic Vapor Laser Isotope System (AVLIS) program. At Lick, green light from solid state lasers beneath the main floor of the telescope travels through fiber optics to a compact dye laser mounted on the side of the Shane telescope. A beam projector then directs the yellow dye laser light up through the atmosphere. At about 100 km, the laser beam hits a layer of sodium atoms created by micrometeorites, which vaporize as they enter the upper atmosphere. The yellow laser light, tuned to 0.589 micrometers, excites the sodium atoms, which then emit this yellow light in all directions, creating a glowing guide star in the upper atmosphere wherever the astronomer needs it.

Some of the light from this artificially created star travels back through the atmosphere into the Shane telescope. There, an adaptive optics system measures and corrects the guide star image for atmospheric distortions caused by air turbulence and temperature changes. Small sensors continuously monitor changes in the direction of light waves from the guide star. The sensors send this information to a computer, which in turn controls the movements of hundreds of tiny actuators attached to the back of a flexible mirror. Moving hundreds of times a second, the actuators deform the surface of the mirror to “smooth out” the image of the guide star.

When the telescope is viewing a celestial object, light from the guide star and the object travel through the same turbulence and receive the same corrections from the deformable mirror. The result is a clearer image of the object as well.

Last year, Livermore scientists, operating the adaptive optics system on Lick’s 1-m telescope, observed objects at visible wavelengths. Using natural stars as guides, they corrected images to the diffraction limit of the telescope. At the end of last year, they moved the adaptive optics to the 3-m telescope and, again using natural guide stars, corrected to its diffraction limit in the near-infrared. The last step was to install the laser under the guidance of Herb Friedman, project scientist for the laser subsystem.

(Top left) The black box, highlighted in white, holds the laser package that Livermore researchers developed for the 3-m Shane telescope at Lick Observatory. (Bottom left) Outdoors, the laser beam can be seen for miles.



(Right) The graph shows the data taken on the Shane telescope in the near infrared (2.1 micrometers) for Lambda Bootis, a nearby star in the same constellation as Arcturus. The vertical axis shows the intensity of light in one pixel, which corresponds to the telescope’s diffraction limit. The smaller bump shows the data gathered with the adaptive optics (AO) system turned off. The second image, taken with the adaptive optics system turned on, shows most of the light concentrated in one pixel. If the image were taken in space, away from the atmosphere, that peak would be about four times higher than it appears here.

According to Olivier, the adaptive optics on the 3-m telescope allow astronomers to resolve objects more than 10 times smaller than before, when viewing in the near-infrared. With the addition of the laser guide star, astronomers are now able to perform these high-resolution observations over a large fraction of the sky. “This combination,” notes Olivier, “makes this system arguably the world’s most powerful tool for high-resolution, near-infrared astronomy.”

Now that the Lick system is up and running, the Livermore team and other UC astronomers are beginning high-resolution, near-infrared observations of star-forming regions, quasars, and other interesting astronomical objects. Preliminary results from this research will be available later this fall.

In addition, based largely upon experience gained in building the Lick system, the Livermore team was recently awarded a contract to build the major components of a laser guide star adaptive optics system for the largest telescope in the world, the 10-m Keck telescope in Hawaii, owned by UC and the California Institute of Technology. This system, scheduled for completion in 1997, will become the world’s most powerful tool for high-resolution near-infrared astronomy as we enter the 21st century.

For further information contact Scot Olivier (510) 423-6483 (olivier1@llnl.gov).

Creating a Guide Star

Laser guide star efforts have generally focused on two methods of creating artificial stars. The first method uses visible or ultraviolet light to reflect off air molecules in the lower atmosphere from fluctuations (Rayleigh scattering), creating a star at an altitude of about 10 km. The other method uses yellow laser light to excite sodium atoms at about 90 km. The sodium-layer laser guide star turns out to be crucial for astronomy, because astronomers need large telescopes to see objects that are very far away and therefore very dim. These large telescopes require the laser guide star to be as high as possible so that the light from the laser star and the observed object pass through the same part of the atmosphere. With a guide star at the lower elevation, the system senses and corrects for only about half of the atmosphere affecting the light from a distant object.

The Laboratory’s key contribution to this field has been the introduction of the sodium-layer laser guide star based on AVLIS dye laser technology. Claire Max, the project’s principal investigator and the current Director of University Relations at LLNL, was a co-inventor of the idea of using a laser guide star in the sodium layer of the atmosphere for astonomical telescopes.

Forensic Science Center Update

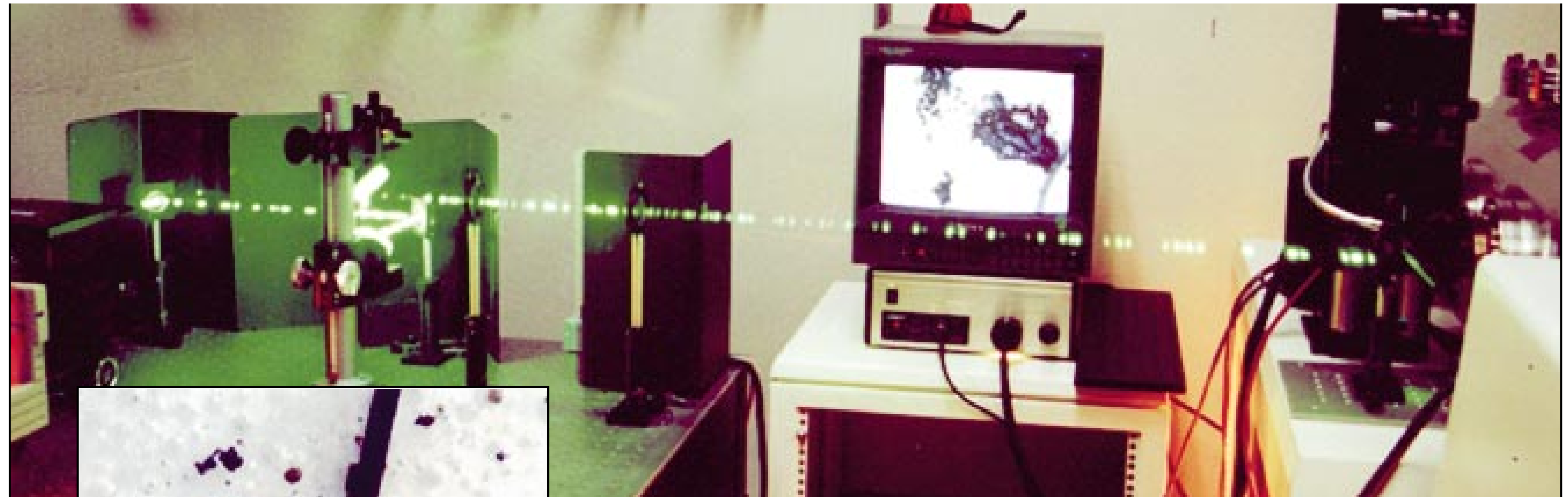
FOR most people, “forensic science” means cops and fingerprints and DNA analysis. All of that is still true, but these days forensic science encompasses much more. Some “whodunits” are more complicated and can involve an international cast of characters. Forensic science now also is used to verify and monitor compliance with such international agreements as the Nuclear Non-Proliferation Treaty and the Chemical Weapons Convention, and to learn whether a country is developing a clandestine nuclear weapons program.

The Laboratory’s Forensic Science Center was established in 1991, and in its short life has become a leader in law enforcement, national security, defense, and intelligence applications. Using sophisticated analytical equipment, experts in organic, inorganic, and biological chemistry can determine the composition and often the source of the most minute samples of material. Lasers are also being used to “interrogate,” or examine, a variety of materials.

The March 1994 issue of *Energy & Technology Review* described in detail the workings of the Forensic Science Center. It reported on the Center’s excellent performance in a “round-robin” series of exercises with analytical chemistry facilities from around the world. The Center has done so well in these exercises over the years that it is no longer just a participant. Its staff also prepares samples for other laboratories to analyze. Following is an update on activities at the Forensic Science Center since early 1994.

What You See Is What You Get

By combining three technologies into a single system—an ion trap mass spectrometer for analysis, a high-powered microscope for viewing, and a laser for ionizing samples—the Center has created something entirely new for forensic analysis: imaging laser-ablation mass spectroscopy. Conceived in 1994 and still being refined, this new process allows considerably more accuracy in analyzing samples than standard mass spectroscopy.



The photo above shows the imaging laser-ablation mass spectrometer system in action. From the left, the 2.5-gigawatt-per-cm^2 Nd:YAG (neodymium yittrium-aluminum-garnet) laser beam is passing through steering and alignment optics in the imaging system and into the mass spectrometer. A display of the target material is visible on the videoscreen. To the left is a magnified human hair after bombardment by the laser beam.

Sampling material is placed on the tip of a probe that is inserted into the source region of an ion trap mass spectrometer. With a microscope outside the vacuum chamber, the sampling material is viewed from above at 250 × magnification. A laser beam is then directed at precisely the 10- to 50-micrometer spot on the probe tip from which the sample’s mass spectral data is desired. The intensity of the laser beam can be adjusted to instantaneously vaporize more or less sampling material, depending on the size of the sample. The laser ionizes the material, and the mass spectrometer sorts these fragments according to their molecular weights. Once sorted, each chemical component produces a characteristic mass spectral fragmentation pattern that is used by the operator to identify the entire sample.

There are several benefits of this method. The new imaging capability allows for a more accurate focus of the laser beam, which means more accuracy in sampling and more accuracy in analysis. By having the sampling material inside the mass spectrometer vacuum chamber before it is hit with the laser beam, sample losses are far less than when the sample is bombarded outside the ion source and then transferred to the mass spectrometer. We can also analyze smaller particles and fibers with this system than we can with a standard bench-top ion trap.

This new system has numerous applications. One possible use is to provide a chronological record of chemical exposures by analyzing hair, vegetation, and other materials. For example, ingestion of or exposure to certain chemicals, including illegal drugs, can be identified in human hair. Since human hair generally grows at about one-half inch per month, analysis of a person’s hair along its length can provide a chronology of drug use over time (see photos above). Or the hair of a dog known to have been kept as a pet at a suspected drug manufacturing facility can be analyzed to determine chemicals associated with chemical spills and exposures at the drug lab. Positive identification of chemicals in the dog’s hair, indicative of the lab’s operations, could serve as criminal evidence in a trial.

Although this technique is still in its infancy, its potential could be enormous. As lasers become easier to use, smaller and smaller particles and fibers will be sampled and characterized in forensic investigations.

Miniaturizing the GC/MS

The Forensic Science Center is also at the forefront in developing new, portable systems capable of real-time analysis in the field. These units have numerous applications, from identifying materials to support verification of the Chemical Weapons Convention to investigating criminal activities.

All of the traveling components of LLNL’s miniaturized gas chromatograph/mass spectrometer can fit into a metal travel case. Included are (on table) the GC/MS and laptop computer and (on floor) the pumping unit and generator.

Almost five years ago, the Center developed a suitcase-size gas chromatograph/mass spectrometer (GC/MS) for on-site identification of ultratrace (microgram or less) quantities of certain compounds in complex mixtures. The system weighed 68 kg (150 lb), which made it portable, but only barely. Three years later, the system’s weight had been cut by more than half to 32 kg (70 lb), still a hefty load. Today, at 20 kg (44 lb), with an accompanying laptop computer, this system can realistically be considered portable. This rugged, all-metal vacuum vessel can be carried on board an airplane and put into the overhead compartment, while its accompanying generator and off-line vacuum reconditioning pumping unit travel in the baggage compartment.

Reduction in size does not mean a reduction in performance. The latest complete GC/MS unit is able to achieve the almost-perfect vacuum required for accurate analysis. It can run for 12 hours in the field, and, like a 500-lb bench-top model, can perform up to 200 operator-assisted analyses per day. While the operator sleeps, the turbomolecular pumping station refreshes the vacuum and other systems in the unit for another 12 hours of operation.

And how have they made this unit so small? When LLNL first took on the job of making a portable GC/MS system, very few off-the-shelf parts were available that, when assembled, would fit into anything the size of a suitcase. Almost all of the pieces that went into the first 68-kg unit were therefore designed and manufactured at LLNL. Meanwhile, miniaturization began to catch on in the GC/MS industry, so many of the components of the 32-kg version could be purchased from outside sources. While a few components of the latest 20-kg model had to be produced here, most have been purchased commercially, modified as necessary, and fitted together.

The unit's hydrogen supply for the portable gas chromatograph is typical of the shrinking components. The hydrogen supply in the 68-kg model weighed 14 kg. Today it weighs just 0.4 kg and still operates at 250 psi, just like its bigger bench-top brother.

The Center also has produced another unit whose parts can be replaced in the field. Parts are fitted together with O-rings, which facilitates repair, but more pumping capacity is needed to hold the desired vacuum. So there is still much work to do.

Counter-Forensic Inspection

In the summer of 1994, DOE asked the Forensic Science Center to perform a preliminary "counter-forensic" analysis to help the government investigate vulnerabilities of two gaseous-diffusion, uranium-enrichment plants that will be subject to international inspections. Although inspections of the plants are expected to be visual only, DOE wanted to know whether a hypothetical inspector with a different agenda, while walking through one of its plants, could surreptitiously collect samples of material, take them home, examine them, and replicate the enrichment process. The Center's mission was to examine the similar samples and learn critical details of the enrichment process.

In the gaseous diffusion enrichment process, uranium hexafluoride passes through a series of semipermeable barriers, the number of barriers being determined by the enrichment required. Uranium used in power reactors requires less enrichment than weapons-grade uranium, which is highly enriched.

The Center used for its analysis a variety of materials collected from different areas in the plant. With minute quantities of these materials and state-of-the-art analytical equipment, our chemists, engineers, and metallurgists were able to determine whether or not various aspects of the enrichment process are vulnerable to surreptitious collections. We expect these results to be useful in determining future inspection protocols.

For further information contact Brian Andresen (510) 422-0903 (andresen1@llnl.gov).

Patents

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Raymond P. Mariella, Jr. **Gregory A. Cooper**	Infrared-Sensitive Photocathode U.S. Patent 5,404,026 April 4, 1995	A single-crystal, multilayer device incorporating an IR absorbing layer that is compositionally different from the $Ga_xAl_{1-x}Sb$ layer, which acts as the electron emitter. Different IR absorbing layers can be used, limited only by the ability to grow quality material on a chosen substrate.
Arnold C. Lange	Base Drive Circuit U.S. Patent 5,404,052 April 4, 1995	Electronic circuitry for controlling bistable switching circuits, particularly high-power circuits for an electron-beam gun or electric motor. The switching control circuit ensures that bipolar power sources are not shorted together. A pair of solid-state output devices are connected to a level shifter through a pair of nonlinear delays.
Blake Myers	Ceramic Tile Expansion Engine Housing U.S. Patent 5,404,793 April 11, 1995	A high-temperature engine housing, including interlocking ceramic tiles that form an expandable ceramic housing; a pressurizable external metal housing that provides a support for the ceramic tiles; and means for thermally insulating the metal housing from the ceramic housing.
Stanley W. Thomas	Image Intensifier Gain Uniformity Improvements in Sealed Tubes by Selective Scrubbing U.S. Patent 5,408,087 April 18, 1995	A microchannel-plate image intensifier having a photocathode that is damaged to reduce high-gain areas. The high-gain sections are selectively scrubbed with a controlled bright light source.
Ronald E. English, Jr. **John J. Christensen**	Optical Power Splitter for Splitting High Power Light U.S. Patent 5,408,553 April 18, 1995	A prism segmenter having a plurality of prisms arranged about a central axis for forming a plurality of divided beams of light from a single beam of light without using complex optical pathways or sensitive components.
Thomas M. Tillotson **John F. Poco** **Lawrence W. Hrubesh** **Ian M. Thomas**	Method for Producing Metal Oxide Aerogels U.S. Patent 5,409,683 April 25, 1995	A two-step hydrolysis-condensation method to form metal-oxide aerogels of any density, including densities of less than $0.003 g/cm^3$ and greater than $0.27 g/cm^3$. A condensed metal intermediate is formed and can be stored for future use.
John S. Toeppen	Method and Apparatus for Holographic Wavefront Diagnostics U.S. Patent 5,410,397 April 25, 1995	A wavefront diagnostic apparatus and method for determining the parallelism of the rays of light within a beam of light by comparing projected and reference holographic images. Other geometric parameters can be measured using these diffractive optical elements.
Mark A. Rhodes	Magnetron Cathodes in Plasma Electrode Pockels Cells U.S. Patent 5,410,425 April 25, 1995	An electro-optic switch using magnetron cathodes as plasma electrodes. A low-pressure ionized gas is formed on both sides of the crystal. A magnetic field is produced by permanent magnets or electromagnets near the surface of the cathode.

Awards

The 1995 R&D Awards were given to five Laboratory groups for 1995 achievements in scientific and technological breakthroughs. Given by the Chicago-based R&D Magazine, *100 of these prestigious awards are presented each year. Following are the technologies and LLNL personnel involved.*

- Sealed Tube Electron Beam Guns for Material Processing: **Booth Myers**, **Hao-Lin Chen**, **James Davin**, and **Glenn Meyer**, and **George Wakalopulos** and **Peter Bond**, American International Technologies, Inc.

- Miniature Ion Cyclotron Resonance Mass Spectrometer: **Daniel Dietrich** and **Robert Keville**.

- All-Solid-State Laser with Diode Irradiance Conditioning: **Raymond Beach**, **Christopher Marshall**, **Mark Emanuel**, **Stephen Payne**, **William Benett**, **Barry Freitas**, **Steven Mills**, **Scott Mitchell**, **Charles Petty**, **John Lang**, and **Larry Smith**.

- High Average Power Solid-State Laser with High Pulse Energy and Low Beam Divergence: **Clifford Dany**, **Lloyd Hackel**, and **Mary Norton**.

- Aerogel Process Technology: A shared award for two different processes (1) Injection Molding Process for Rapid Production of Net-Shaped Aerogels: **Lawrence Hrubesh**, **Paul Coronado**, and **John Poco**. (2) Capacitive Deionization with Carbon Aerogel Electrodes: **Joseph Farmer**, **Richard Pekala**, **David Fix**, **Gregory Mack**, **John Poco**, **William Grant**, and **Charles Pomernacki**.

The Laboratory received a 1995 National DOE Pollution Prevention Award for achievement in recycling hazardous materials. Specifically recognized were eight employees in Plant Operations that received the National Award for Radioactive/Hazardous Waste Recycling. They are **Keith Gilbert**, **Mike Hayes**, **Rod Hollister**, **Charlie Patterson**, **Linda Souza**, and **Robert Wiebers**. The Laboratory's Hazardous Waste Management's CHemical Exchange Warehouse (CHEW) received a special mention, as did its developers **Marjorie Gonzalez** and **Mike DeMicco**.

Scanning Tunneling Microscopy: Opening a New Era of Materials Engineering

Incorporating an STM into an ultra-high-vacuum environment that contains a suitable combination of facilities for sample preparation, material deposition, and complementary diffraction-based surface diagnostics has enabled us to analyze the atomic details of the growth of a variety of thin films for diverse applications. We are currently applying this combination of techniques to evaluate how processing parameters, such as substrate temperature and film deposition rate, affect the atomic structures of interfaces in the fabrication of multilayers for x-ray optics, microelectronics, and magnetic recording devices. The results of these studies allow us to identify the surface defects that have a critical influence on film growth, to investigate their origins, and ultimately to control their occurrence. By doing so, we can improve new materials and devices and give them better performance characteristics.

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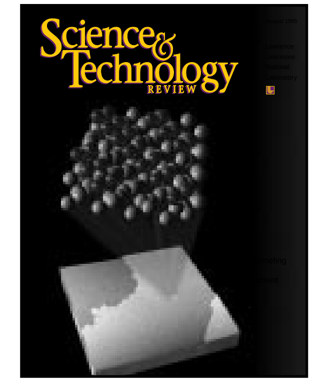
Peter J. Bedrossian (510) 423-5938 (bedrossian1@llnl.gov).

Risk Assessments: From Reactor Safety to Health Care

The Laboratory's Fission Energy and Systems Safety Program (FESSP) performs engineering risk assessments to study and assess the safety, reliability, and effectiveness of various products, processes, and facilities. Evolving methods and techniques are discussed in the context of four cases: an analysis to develop seismic criteria for siting and design of nuclear power plants, risk analysis of reactor coolant piping systems to establish new piping design objectives and increase nuclear power plant safety, study of risks involved in the transport of spent reactor fuel to determine the level of safety provided during transport and the adequacy of existing transport regulations for such material, and development of an approach to identify human-initiated risks in the use of nuclear medical devices such as the Gamma Knife.

■ ***Contact:***
Edwin Jones (510) 422-8259 (jones37@llnl.gov).

U.S. Government Printing Office: 1995/683-074-20017



Science & Technology Review FAX Survey

What Do You Think?

This issue of *Science and Technology Review* (formerly *Energy and Technology Review*) represents a modified approach to communicating the work of the Laboratory. The intent of our changes is to make this publication more interesting to a broader audience. Please give us your reactions to our changes by answering the questions in section 1 and 2 below and faxing them back to us at (510) 422-8803. You can also mail your response to the address below. If you photocopy this form first, you won't have to remove it from the publication.

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Risk Assessments	❑	❑	❑	❑
Guide Star/Lick Observatory	❑	❑	❑	❑
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Scanning Tunneling Microscopy	❑	❑	❑	❑
Risk Assessments	❑	❑	❑	❑
Guide Star/Lick Observatory	❑	❑	❑	❑
Forensic Science Center	❑	❑	❑	❑

How interesting and valuable do you find our new sections?

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The Laboratory in the News	❑	❑	❑	❑
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